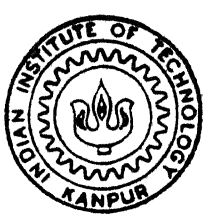
A MODEL FOR THE PREDICTION OF Ae_3 TEMPERATURE OF MULTICOMPONENT STEEL

by

MANOJ KUMAR



DEPARTMENT OF MATERIALS AND METALLURGICAL ENGINEERING

INDIAN INSTITUTE OF TECHNOLOGY KANPUR

JULY, 1994

A MODEL FOR THE PREDICTION OF Ae_3 TEMPERATURES OF MULTICOMPONENT STEEL

A Thesis Submitted
in Partial Fulfilment of the Requirements
for the Degree of

MASTER OF TECHNOLOGY

by

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to the

DEPARTMENT OF MATERIALS AND METALLURGICAL ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY, KANPUR

JULY, 1994

CERTIFICATE

Certified that the work reported in this thesis entitled 'A Model For The Prediction Of Ae_3 Temperatures Of Multicomponent Steel' by Mr. Manoj Kumar has been carried out under my supervision and has not been submitted elsewhere for the award of a degree.

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ACKNOWLEDGEMENTS

I wish to express my deepest sense of gratitude and sincere regards to Dr. A. K. Jena for his invaluable guidance and constant encouragement in the successful completion of this work.

I express my gratitude to Mr. Rajneesh Singh who constantly helped me in writing this thesis. I also wish to thank my friends - Rajesh Khanna,Sameer Joshi , Amod Kumar, Brijesh Dixit, Sunil Kumar. Amit Nagar. Balwinder Bhatia and others, who apart from making my stay at the Institute very pleasant and memorable, also helped me in innumerable ways from time to time.

I also wish to thank to Mr. S. Chaudhary and Mr V. Kumar for helping me at various occasions.

MANOJ KUMAR

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LIST OF SYMBOLS

G	Gibb's free energy
H	Enthalpy
R	Universal gas constant
α	Ferrite
γ	Austenite
T	Temperature
e	Equilibrium
W_i	Weight percentage of an element i
X_i	Weight fraction of an element i
SE	Standard error of estimate
SOSR	Sum of squared residuals
α	Significance level

ABSTRACT

An attempt was made to correlate Ae_3 temperatures with composition of steels containing upto seven components. 177 accurately determined data points were selected from the literature. The Ae_3 temperatures and the corresponding steels compositions were recorded. A relation between Ae_3 temperature and steel composition was developed. The data available on seven binary systems, Fe-C, Fe-Mn, Fe-Si, Fe-Ni, Fe-Cr, Fe-Mo and Fe-Cu, were curve fitted and the relations were obtained which yielded maximum error of estimate , $\sigma = \pm 2.48^{o}C$ in the case of Fe-C . For multicomponent steels, two cases were considered. In one case, binary coefficients of Si were fixed and in other case no coefficients were fixed. For both cases, different sets of significance levels were considered and the best results were accepted. It was found that the both cases gave equally satisfactory results.The model developed in this investigation yields results that are far better than those predicted by the three models available so far in the literature.

CHAPTER I

INTRODUCTION

Steel is an important material that has numerous applications. Its properties depend on various factors such as chemical compositions,different processing parameters that give rise to various metallurgical structures etc. Heat treatment is an important metallurgical process by which properties of various kind of steels can be controlled and monitored. Ae_3 temperature is an important parameter whose knowledge is essential for the heat treatment if properties are to be monitored effectively.

Ae_3 temperature can be determined experimentally. But Ae_3 temperature changes with change in composition and components of steel. Different compositions have different Ae_3 temperature. Generally, steels with wide variation in composition and with components are used extensively. Therefore ,it becomes impractical to carry experimentation for each steel to determine its Ae_3 temperature. It is in this context that mathematical models show their suitability. Importance of Ae_3 temperature can be gauged from the fact that many mathematical models exist to predict the Ae_3 temperature. The problem with these models is that they are not very accurate. Hence the need arise to develop a better model and thus justifying the present work. In the present work,attempt has been made to mathematical equations to predict the Ae_3 temperature for seven binary systems and multi component systems containing up to seven components which include C,Mn,Cu,Ni,Mo,Cr and Si. Polynomial curve fitting techniques as well as step-wise linear regression

techniques have been used. The results show considerable improvement compared with the predictions of models available in the literature.

CHAPTER II

LITERATURE REVIEW

2.1 Fe-C Phase Diagram:

Many investigations have been carried out to establish phase relationship in the iron-carbon system. Different metastable phases have been found to exist due to small different differences in Gibbs Free Energy of the metastable and corresponding stable phases. However, here aim is not to discuss those features of the phase diagram. We are mainly interested in the Ae_3 temperature in the diagram. Ae_3 temperature expresses the temperature at which an iron-carbon alloy, with composition less than the eutectoid composition, will start converting into ferrite while cooling or will start converting into austenite while heating. This particular temperature is referred as Ae_3temperature. Ae_3 line commences from the point where pure γ-Fe converts into α-Fe and ends at the eutectoid point. This eutectoid point is affected if the eutectoid composition represents the metastable equilibrium among austenite, ferrite and cementite instead of the stable equilibrium among austenite,ferrite and graphite. However, metastable or stable equilibrium does not change the Ae_3 temperature. The Fe-C phase diagram[1] showing the Ae_3 temperature is given in Fig.2.1.

2.2 Binary Phase Diagram with Substitutional Alloying Elements:

Binary phase diagram of iron with Mn,Cr,Ni,Mo,Si and Cu which have been published with the latest available data are reproduced in figures 2.2 to 2.7.

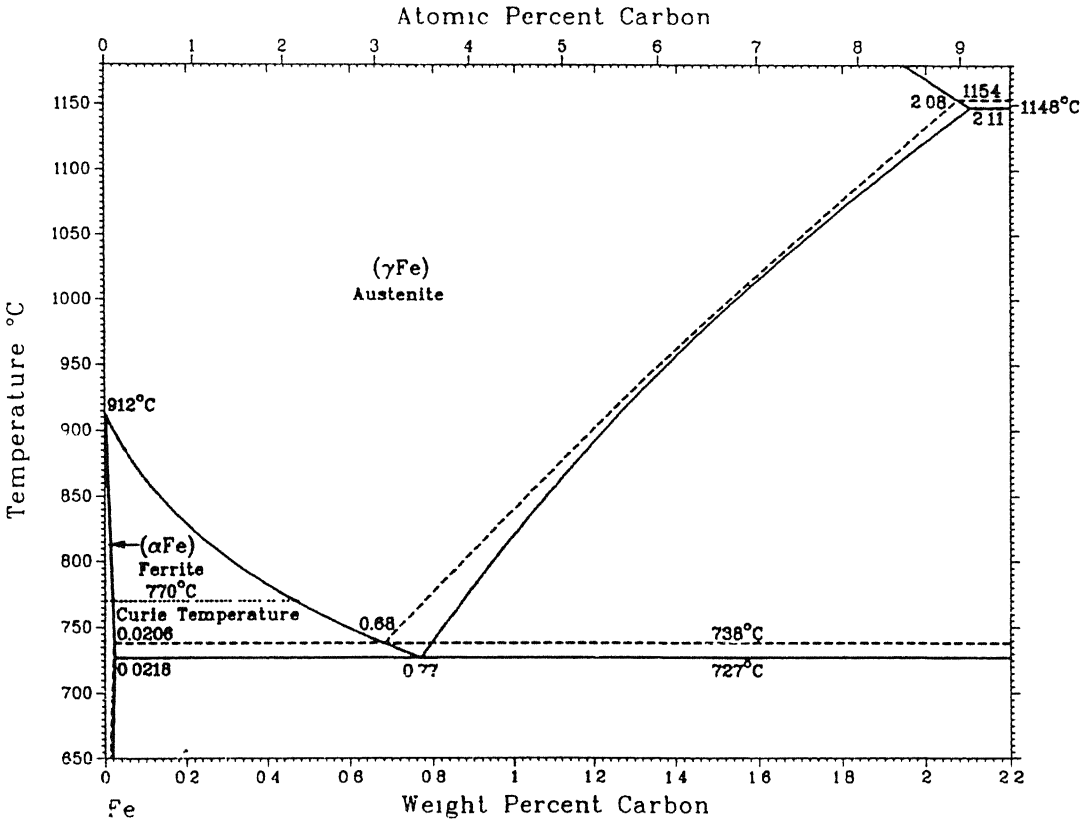


Fig.2.1 Fe-C Phase Diagram

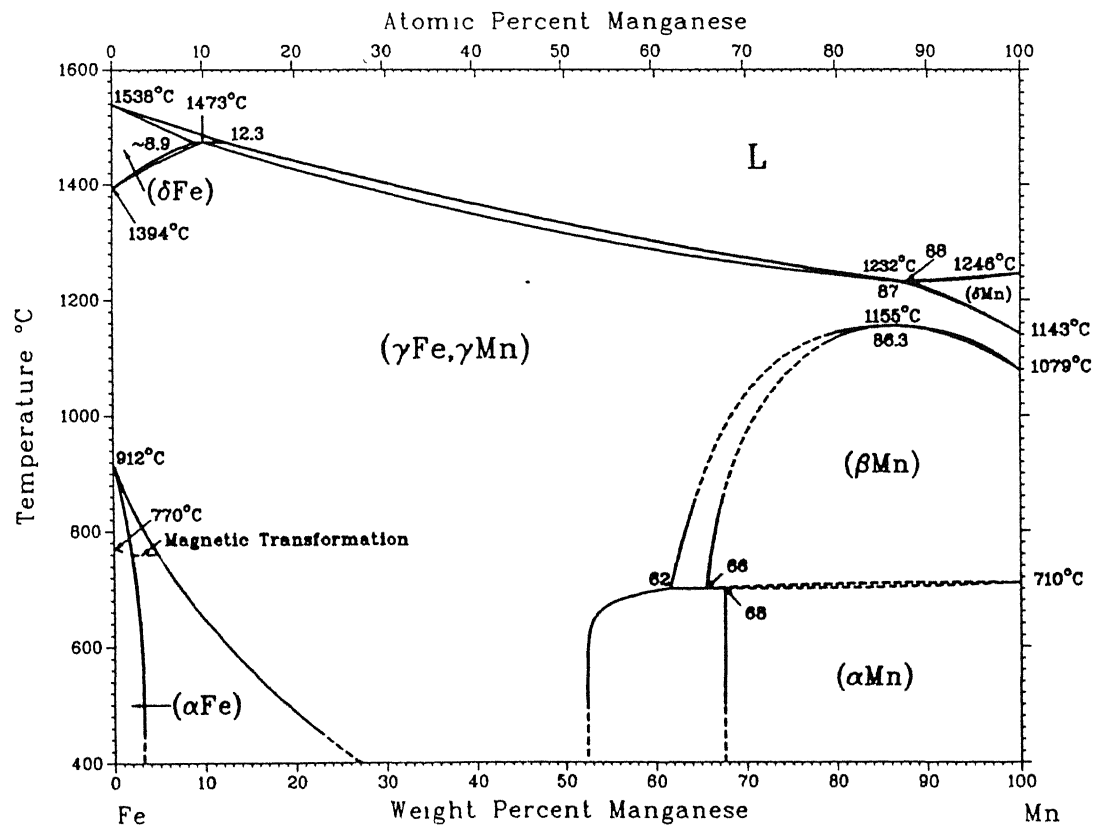


Fig.2.2 Fe-Mn Phase Diagram

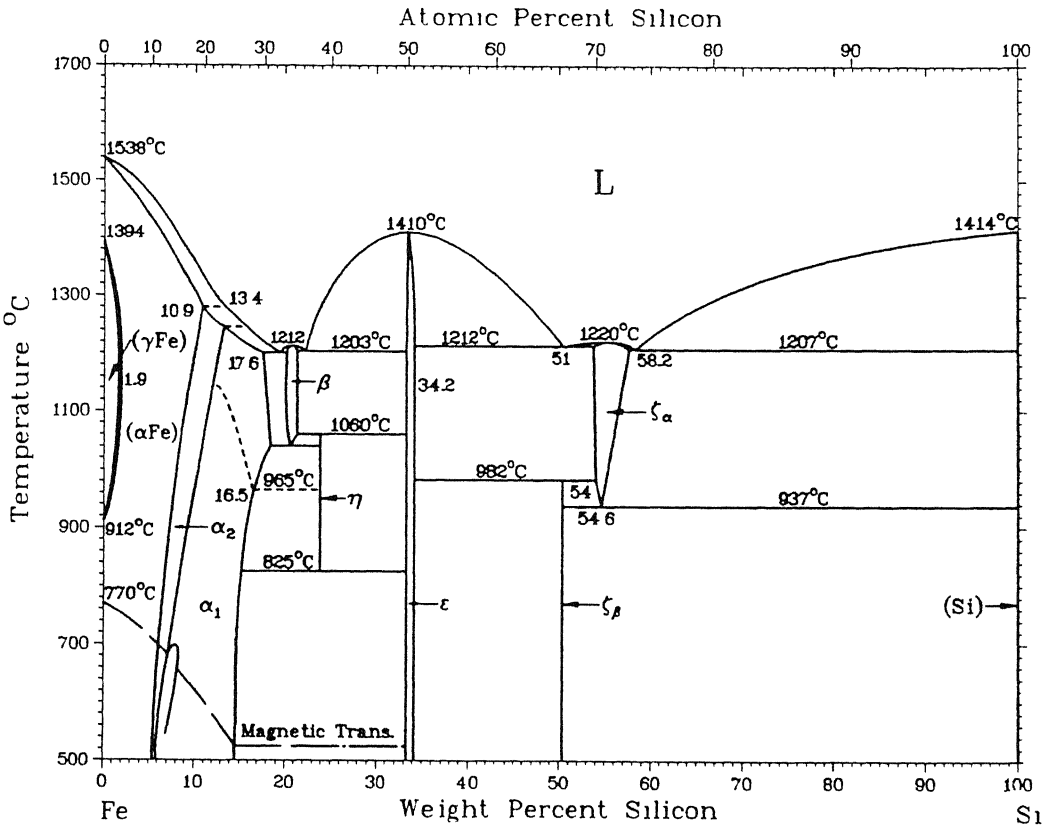


Fig.2.3 Fe-Si Phase Diagram

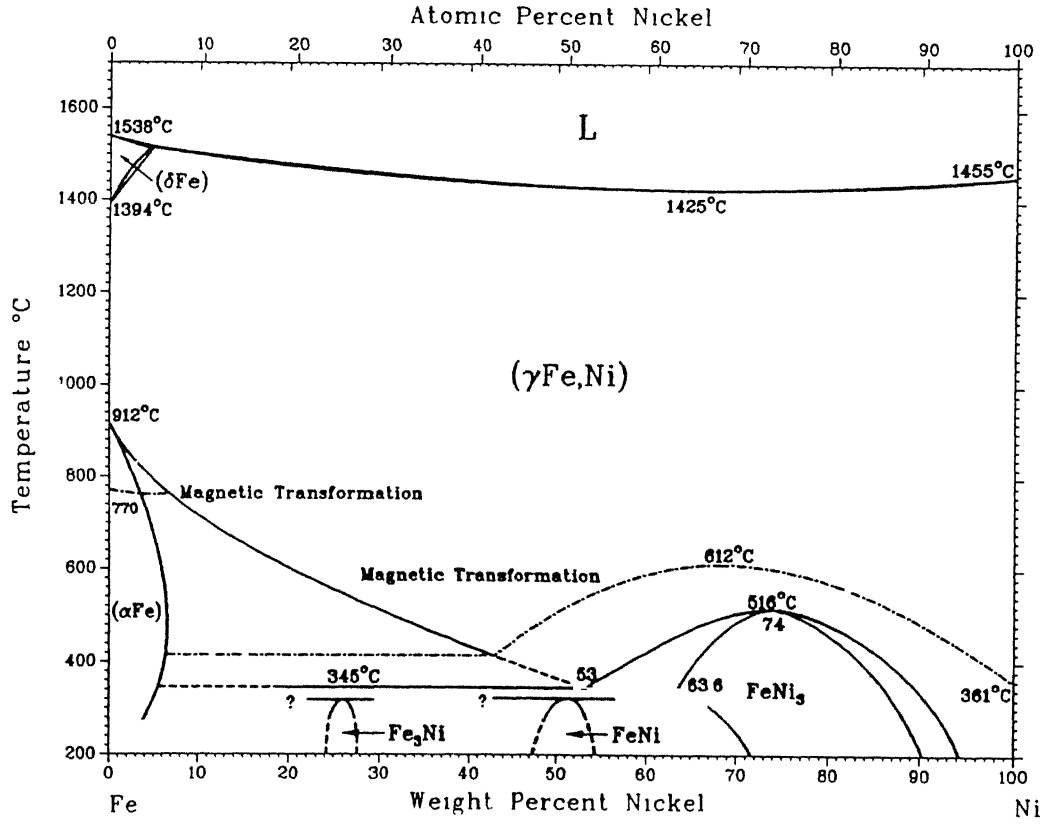


Fig.2.4 Fe-Ni Phase Diagram

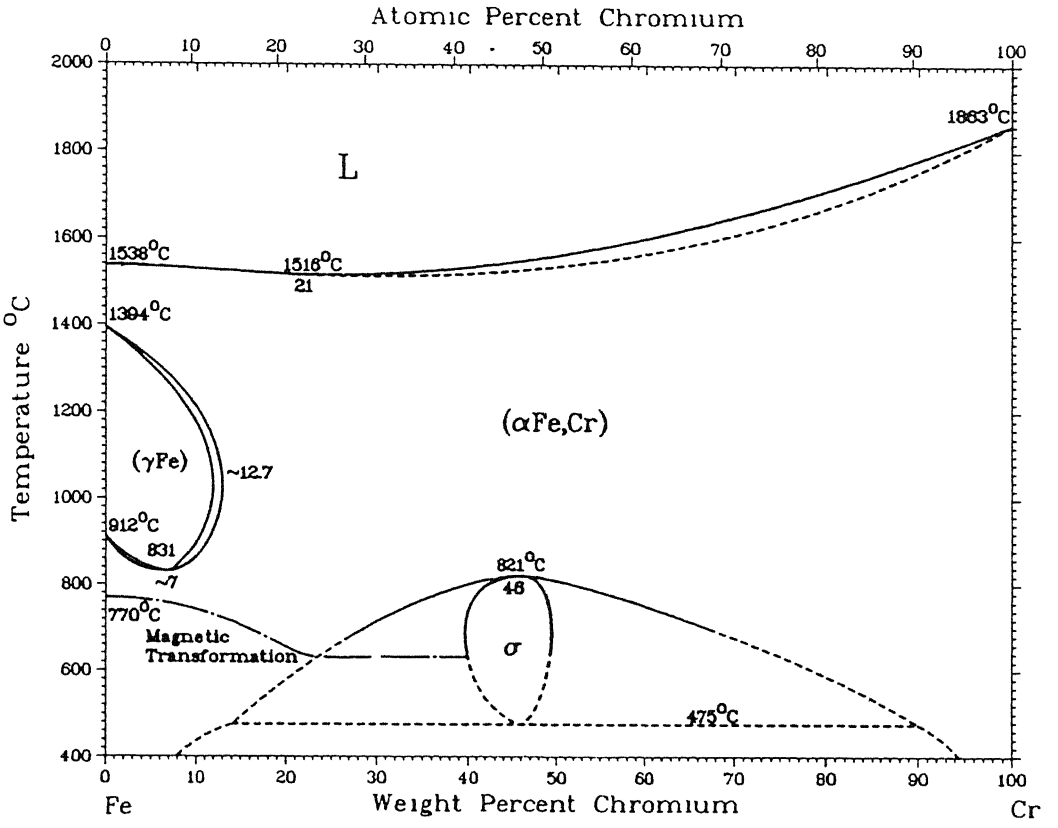


Fig.2.5 Fe-Cr Phase Diagram

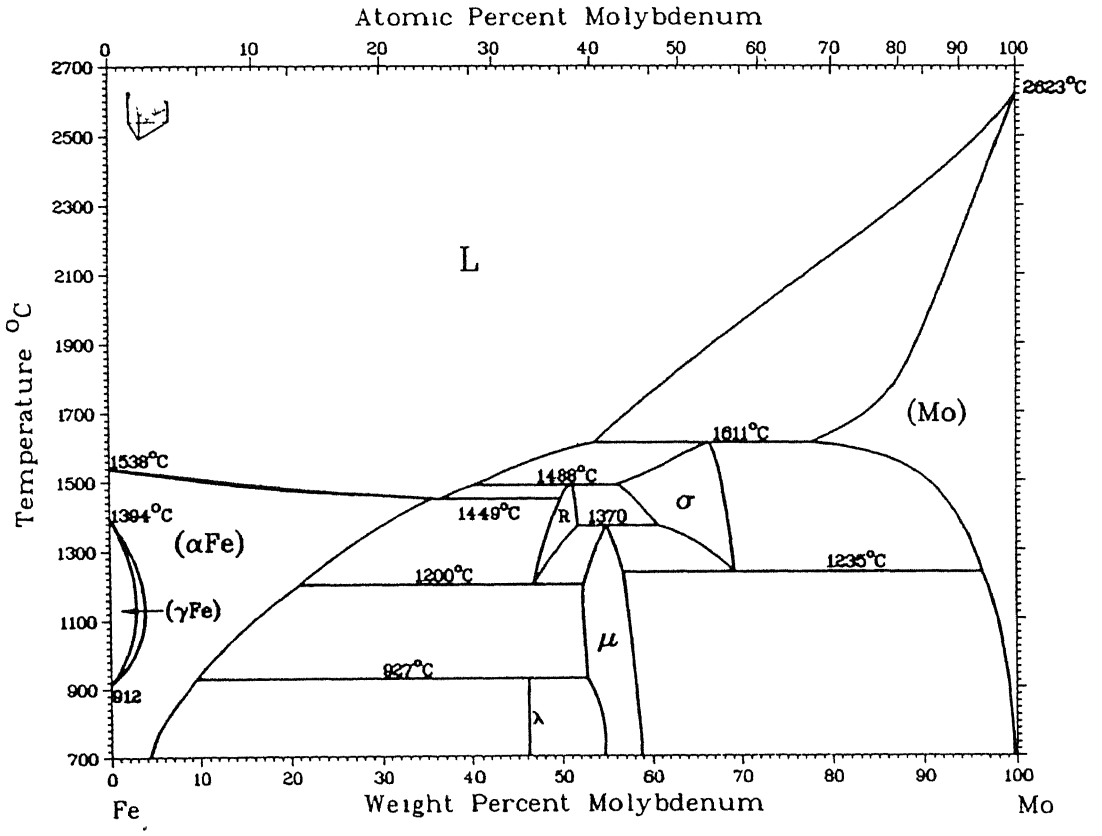


Fig.2.6 Fe-Mo Phase Diagram

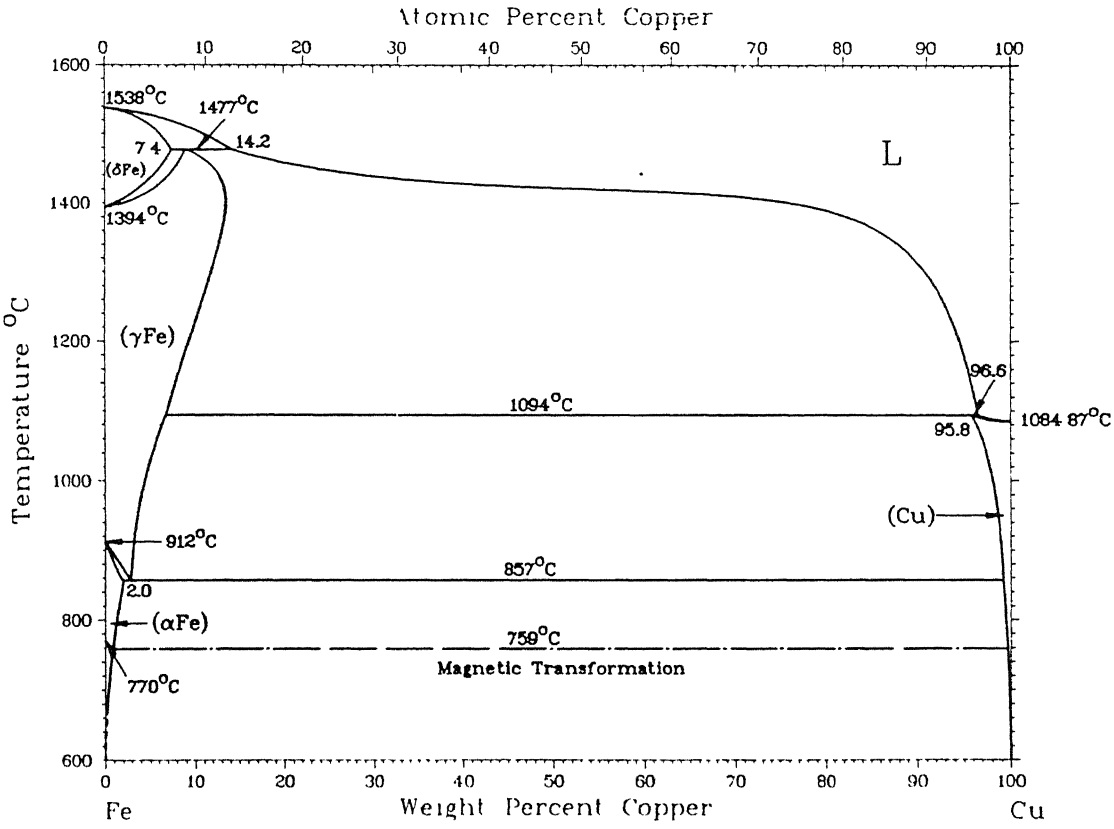


Fig.2.7 Fe-Cu Phase Diagram

Iron-manganese diagram is taken from Massalaski et. al [1], however, it has been redrawn from Kubaschewski [2]. Fe-Cr phase diagram is taken from Massalski et. al [1] ,however, it has been redrawn from [3]. Fe-Cu diagram is taken from Massalski et. al [1], however, it has been redrawn from Kubaschewski [2]. Fe-Mo diagram is taken from Massalski et. al [1], however, it has been redrawn from [4]. Fe-Ni diagram is taken from Massalski et. al [1], however, it has been redrawn from Kubaschewski [2]. Fe-Si diagram is taken from Massalski et. al [1], however, it has been redrawn from Kubaschewski [2].

2.3 Effects of Alloying Elements on Fe-C Phase Diagram:

The elements that enhances the properties of the steel are are generally referred as alloying elements. These are Mn,Cr,Ni,Co etc. Some elements that affect the properties adversely are known as impurities, such as phosphorus and sulphur. Both alloying elements and impurities modify the phase diagram features. Alloying elements present in a steel may increase or decrease a particular phase field in the Fe-C phase diagram. These elements change the boundaries of the phase fields and thus affecting the various phase transformation temperatures of of a steel. The elements also affect the various critical temperatures e.g eutectoid transformation temperature. The effects of impurities on the phase diagram is similar to those of alloying elements. The elements that expand the austenite region are known as austenite stabilizers. Those that expand the ferrite field are known as ferrite stabilizers and those that increase the carbide stability are referred as carbide stabilizers. Thus by selecting one or more alloying elements one can make a phase say,

austenite to be stable over wide range of temperatures. Thus , austenite can be made stable even at low temperature . The elements such as Mn,Ni,Cu,Co,C are the austenite stabilizers. And Cr,Si,Mo,Ti are ferrite stabilizers. Austenite stabilizers decrease the Ae_3 temperature whereas ferrite stabilizers increase it. The addition of alloying elements change the temperature at which gamma iron transforms to alpha iron. The alloying elements also alter the eutectoid transformation temperature. The effect could be either increase or decrease in the temperature depending on which elements are added. The eutectoid composition may also be changed by the alloying elements. Ti, Mo, Si, Cr increase the eutectoid temperature whereas Mn and Ni decrease it. Although the effect is not linear with the composition of the alloying elements . The elements such as Ti , Mo, Si, Mn, Cr, Ni decrease the carbon composition at which eutectoid transformation takes place. Although effect is not similar for all these elements. For example, Ti decrease the composition drastically. The behaviour is not similar for the entire composition range of an element. For example, in the case of Mo, the eutectoid composition increases after certain composition of Mo.

2.4 Data Available on Ae_3 Temperature:

Ae_3 temperature of only a limited number of multicomponent steels have been detemined experimentally. Grange [5] has reported the Ae_3 temperature of nineteen steels. THe Unite States Steel Corporation [6]has published isothermal transformation diagrams for several steels from which the Ae_3 temperatures can be obtained. Aaronson and Domian [7] and Hall et. al [8] have also reported Ae_3 temperatures for a few steels. Gilmour et. al[9] and Kirchner and

Uhrenius [10] have reported the compositions of ferrite and austenite in equilibrium at different temperatures. The composition of the austenite in equilibrium with ferrite at a particular holding temperature can be taken to be the composition of steel having Ae_3 temperature equal to the holding temperature. The atlas of the isothermal and continuous transformation diagrams [11] give Ae_3 temperature of several steels. Ae_3 temperatures of binary systems like Fe-C, Fe-Mn, Fe-Si, Fe-Ni, Fe-Cu, Fe-Cr,Fe-Mo can be obtained from the corresponding binary equilibrium diagrams review in section 2.2.

2.5 Available Models for Predicting Ae_3 Temperature:

A number of models are available in the literature. These are those of Grange[5] ,Andrews[12] and Baganis[13].

Grange's Model[5]: Grange[5] has based his model on experimental data on nineteen steels. He has suggested the following model for prediction of Ae_3 temperature, T_e (in ^oC) :

$$T_e = 854.4 - 179.4X_C - 13.9X_{Mn} + 44.4X_{Si} - 17.8X_{Ni} - 1.7X_{Cr}$$

Where X_C, X_{Mn}, X_{Si}, X_{Ni} and X_{Cr} represent the weight percentage of the alloying elements.

Andrews Model[12]: Andrews[12] Also based his on Grange's [5] data on nineteen steels. His model is:

$$T_e = 913 - \Delta T - 25\,X_{Mn} - 11\,X_{Cr} - 20\,X_{Cu} + 60\,X_{Si} + 60\,X_{Mo} + 40\,X_N + 100\,X_V + 700\,X_P$$

Here ΔT accounts for the effects of carbon and nickel on Ae_3 temperature. ΔT is dependent on the equivalent carbon content which is obtained by adding one tenth of the weight percentage of nickel

to the weight percentage of carbon. The value of ΔT is obtained from the following data:

$X_C + (X_{Ni} / 10)$:	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40
ΔT (^{o}C) :	24	48	64	80	93	106	117	128
$X_C + (X_{Ni} / 10)$:	0.45	0.50	0.60	0.70				
ΔT (^{o}C) :	137	145	160	170				

Baganis's Model[13]: Baganis[13] calculated the Ae_3 temperatures using the published data on free energy and activity of binary and ternary alloys of iron. His model is:

$$T_e = T_o + \Delta T$$

Where

$$\Delta T = R\, T^2 \, \Sigma \, X_{i,\gamma} \, [\, A\, B \,] \,/\, [\, C\, D]$$

and

$$A = \left(\frac{\Delta G_i (T_0)}{R\, T_0} + E_{1i}\, X_{1,\gamma} \right) - \left(1 + e_{1i}\, X_{1,\gamma} \right)$$

$$B = \exp\left\{ \frac{\Delta G^{o}_{o} (T_o)}{R\, T_o} - \frac{e_{11}}{2} \left(X_{1,\gamma} \right)^2 \right\}$$

$$C = \left(1 - X_{1,\gamma} \right) \Delta H^{o}_{o}$$

$$D = \exp\left\{ \frac{\Delta G^{o}_{o} (T_o)}{R\, T_o} - \frac{e_{11}}{2} \left(X_{1,\gamma} \right)^2 \right\}$$

T_o = Ae_3 temperature of plain carbon steel.

$X_{1,\gamma}$ = mole fraction of the i^{th} alloying element in γ .

$\Delta G_i^o(T_o)$ = change in the partial molar Gibbs free energy of the i^{th} transformation element at temperature T_o for ferrite to austenite

E_{1i} = interaction coefficient for the solute i and carbon in iron

ΔH_o^o = change in the partial molar enthalpy of iron for ferrite to austenite transformation

In the expression for T , suffix 0,1,...,i,...,n of G, H and e indicate the constituents. 0 stands for iron , 1 for carbon and 2 to n for other substitutional alloying elements.

2.6 Curve Fitting Technique:

In curve fitting, attempt is made to find an analytic expression of the form y = f(x), for the functional relationship suggested by the given data. It has considerable importance both in theory and practice. Theoretically, it is useful in the study of correlation and regression. In practice it enables us to represent the relationship between two variables by simple algebraic expressions, e.g, polynomials, exponential or logarithmic functions. Once we have the relationship between two variables we can predict the influence of the independent variable on the dependent variable. Selection of a particular mathematical relation depends on the trend suggested by the given set of data points. Considerable skill, intelligence and expertise is required for the purpose. One may start with a simple relationship. If no of variables involved are only two then by plotting the given points one may infer the relationship. Then the problem reduces to finding the parameters that give the most suitable fit for the given data points. The concepts of the curve fitting can be extended to the case when more than one independent variables are present. Although in such cases,

we do not have any visual aid to see the trend of the relationship between dependent and independent variables.

2.6.1 Linear Regression:

If the dependent variable y is influenced by p independent variables $X_1,\ldots,X_p$ and has m+1 parameters $b_0, b_1,\ldots,b_m$ and if we represent the functional relation as:

$$y = f (b_0, b_1,\ldots,b_m, X_1, X_2,\ldots,X_p)$$

Then there the following three possibilities:

(i). y is linear with respect to both independent variables and parameters and then the relation can be expressed as:

$$y = b_0 + b_1 X_1 + b_2 X_2 + \ldots + b_p X_p$$

(ii). y is linear w.r.t parameters but nonlinear w.r.t the independent variables in case of one independent variable :

$$y = b_0 + b_1 X + b_2 X^2 + \ldots + b_2 X^p$$

(iii). y is nonlinear w.r.t both parameters and independent variables. One example is :

$$y = e^{b_1 X_1} + e^{b_2 X_2}$$

But only those cases come under the linear regression where the functional relationship is linear with respect to the parameters; it may or may not be linear with respect to the independent variables. If it is linear also with respect to the independent variables then it is known as simple linear regression analysis.

2.6.2 Simple Linear Regression Model:

We express the Y_i (observed value of the dependent variable corresponding to the i^{th} set of independent variables) in the form:

$$y_i = \mu_i + \varepsilon_i$$

Where μ_i is the mean of the i^{th} historical population of the dependent variable that we could have observed when the values of independent variables are $X_{i1}, X_{i2}, \ldots, X_{ip}$. We assume that the μ_i's follow the following relation:

$$\mu_i = \beta_o + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p$$

The reason, as already pointed out earlier, that we call this model a linear regression model is that the equation expresses μ_i as a linear function of the parameters $\beta_0, \beta_1, \ldots, \beta_p$. This equation is simple linear as it is linear with respect to the independent variables also. This model says that the ε_i's are the error terms that cause the observed dependent variable to deviate. Estimate of the Parameters: Once we assume the existence of a mathematical relation then the next step is to estimate the parameters in the mathematical equation. Several criteria can be used to estimate the parameters such as least square point estimate where sum of the residuals is minimized, minimization of the sum of the absolute values of the residuals etc.

Least Square Point Estimate: In this method sum of the squared residuals is minimized to estimate the parameters of the mathematical relation.

Sum of the squared residuals, $SSE = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$

Where y_i = observed value

$\hat{y}_i$ = value predicted by the equation

The estimates of $\beta_o, \beta_1, \ldots, \beta_p$ by least squared residuals as $b_0, b_1, \ldots b_p$ are called least square point estimate.

For SSE to be minimum,

$$\frac{\partial\ SSE}{\partial\ b_0} = -\ 2 \sum_{i=1}^{n} \left(y_i - b_0 - \sum_{j=1}^{p} b_j X_{ij} \right) = 0$$

$$\frac{\partial\ SSE}{\partial\ b_k} = -\ 2 \sum_{i=1}^{n} \left(y_i - b_0 - \sum_{j=1}^{p} b_j X_{ij} \right) X_{ij} = 0$$

For $k = 1, 2, \ldots, p$

Rearranging we get

$$n\ b_o + \sum_{j=1}^{p} b_j \sum_{i=1}^{n} X_{ij} = \sum_{i=1}^{n} y_i$$

$$b_o \sum_{i=1}^{n} X_{ik} + \sum_{j=1}^{p} b_j \sum_{i=1}^{n} X_{ij} X_{ik} = \sum_{i=1}^{n} X_{ik}\ y_i$$

Where $k = 1, 2, 3, \ldots, p$

These p+1 equations are called the 'Normal Equations' and can be solved simultaneously to give the values of b_o , b_1 ,...,b_p.

The reason we prefer to estimate the coefficients by least square method is the Guass-Markov theorem which states that the variance of the population of all possible least square point estimates of β_j is smaller than the variance of the population of all possible point estimates of β_j that could be obtained by using any other unbiased linear estimation procedure.

2.6.3 Linear Polynomial Regression Model:

We express y_i (observed value) in the form:

$$y_i = \mu_i + \epsilon_i$$

Where μ_i is the mean of the i^{th} historical population of the dependent variable that we could have observed for X_i value of the independent variable and ϵ_i is the error term that cause the observed value of the dependent variable to deviate from the mean.

We assume the mean follow the following relationship:

$$\mu_i = \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \ldots + \beta_p X_i^p$$

This is the p^{th} order linear polynomial model in one independent variable.

Interaction: Multiple regression models often contain interaction variables. We say that there is no interaction between two independent variables if the relationship between the mean value of the dependent variable and each one of the independent variables is independent of the value of the other independent variable. There is said to be interaction between two independent variables if the relationship between the mean value of the dependent variable and one of the independent variables is dependent on the value of the other independent variable.

2.6.4 Stepwise Regression:

If we are attempting to choose an appropriate set of independent variables from a large number of potential independent variables, comparing all reasonable models can be quite unwieldy. In this case, it is useful to employ a screening procedure that can be used to identify one set of the most important independent variables. Stepwise regression is one of such screening procedure to do this job. Stepwise regression uses t_{b_j} statistics to determine the importance of the independent variables in various regression models. The t_{b_j} statistics indicates that the independent variable X_j is significant if and only if the related probability value is less than α .

Stepwise Regression Procedure: First, we have to decide the value of α_{entry} (significance level for entering an independent variable in the model) and α_{stay} (significance level upto which an independent variable can stay in the model). The common practice is to choose both as 0.05 . Regarding the choice of α_{entry} and α_{stay} , Draper and Smith [14] suggested that it is usually the best to set α_{entry} equal to α_{stay}.

Step 1: Since we have p independent variables, we consider p models. For each model,

$y = \beta_0 + \beta_1 X_j + \epsilon$

we choose the one having the largest t_{b_j} statistics. We retain that variable in this step.

Step 2: It considers (p-1) possible regression models of the form:

$y = \beta_0 + \beta_1 X_{[1]} + \beta_2 X_{[2]} + \varepsilon$

It is checked whether $X_{[1]}$ should be allowed in the model or not. If it is found that it is significant then both are retained for step 3.

Further Step: The process continues till no variables that are not in model are having t_{b_j} statistics indicating that they are significant at the level of α_{entry} .

Testing the Importance of an Independent Variable: The independent variable X_j is significantly related to the dependent variable y in the regression model if X_j is important or useful in describing, predicting or controlling when using this regression

model. It would seem reasonable to decide that the independent variable X_j is significantly related to the dependent variable y in the regression model if we can , at a high level of confidence reject the null hypothesis $H_0 : \beta_j = 0$ in favour of the alternative hypothesis $H_1 : \beta_j \neq 0$.

2.6.5 Measuring the Utility of the Overall Regression Model: Multicollinearity: It is said to exist when the independent variables in a regression model are interrelated or are dependent on each other.

The hypothesis test of $H_1 : \beta_j = 0$ vs $H_1 : \beta_j \neq 0$ where β_j is the regression parameter is useful in assessing the importance of the single independent variable X_j and therefore in deciding whether to include X_j in the final regression model. However, the problem of multicollinearity, which exists when the independent variables in a regression model are related to each other can hinder the ability of the hypothesis test of $H_0 : \beta_j = 0$ vs $H_1 : \beta_j \neq 0$ to tell whether or not an independent variable is important . Consequently, there is need to develop measures of the combined importance of all the independent variables in a regression model. Multiple correlation coefficients , multiple coefficient of determination etc are such quantities that measure the overall utility of a regression model. If the value of the multiple coefficient of determination is 0.95 , then this means that the regression model explains 95% of the total variation in the model.

2.7 Scope:

The different models available in the literature suffer from

one or other demerits . They do not predict Ae_3 temperature very accurately. For example, Grange's model assumes linear relationship between the weight percentages of alloying elements and the Ae_3 temperature. The interaction between alloying elements has been ignored in this model. Andrews, who suggested a modified model, considered self interaction of carbon and nickel and interaction between carbon and nickel but ignored other interaction. Andrews model becomes less accurate for Mn > 1.0% and Si > 0.8 %. Beyond these limits of the alloy content, the interactions become important.

Baganis[13] considered equilibrium between ferrite and austenite in steels containing Mn, Ni, Cr, Mo, Cu and calculated the Ae_3 temperature using the published data on free energy and activity of binary and ternary alloys of iron. Baganis[13] has taken into account the self interaction of carbon and interaction of carbon with other alloying elements. But he has ignored the interactions among the substitutional alloying elements and self interactions of these alloying elements. His model becomes less accurate for steels with higher alloy contents. He has developed a computer program for calculating Ae_3 temperature taking into consideration self interactions of the substitutional alloying elements but the interactions among the substitutional alloying elements have been ignored in the calculation. The drawbacks of this model are that the model is bulky and to use this model a large number of accurate thermodynamic data is required. Any error in the selection of data may get multiplied in the model due to the exponential functions involved. Analytical expressions for Ac_3 temperature are available

but they can not be used for predicting Ae_3 temperature.

Thus we observe that all the available models contain some drawbacks. Thus there is scope for improvement in the existing models. Thus justifying the need for further work on the model for prediction of Ae_3 temperature.

CHAPTER III

Analytical Representation of Ae_3 Temperature of Binary Alloy Of Iron

3.1 Data for the Binary Alloy of Iron:

Data was obtained from the binary phase diagrams of these alloys[1]. These diagrams had been determined by assessing all the available data in the literature. The data are listed in Table 3.1.

3.2 Curve Fitting Technique:

Linear polynomial regression model was used for the analytical representation of the Ae_3 temperature for the various binary alloys of iron.

A p^{th}- order polynomial regression model can be represented by the following equation:

$$y_i = \beta_o + \beta_1 X_i + \beta_2 X_i^2 + \ldots + \beta_p X_i^p$$

Method of least square point estimate can be used to estimate the various parameters β_o ,$\beta_1$etc of the model.

To decide the order of polynomial to be fitted, one should take into account the the number of data points available to ensure that there is sufficient degree of freedom for the model. Another statistical quantity is standard error which helps in deciding the order of polynomial that is to be retained finally.

A standard package ' MINITAB ' which is a statistical package was used to obtain the required analytical representation of the various binary alloys of iron. Some of the statistical quantities that helped in evaluating a model are described below:

Standard Error of Estimate: It is also called the standard deviation of estimate. It is used to attain a measure of how closely the

Table 3.1

Ae_3 Temperature and Residue of Binary Systems

System	Composition (Wt%)	Expt. Ae_3 Temp. (^oC)	Calc. Ae_3 Temp. (^oC)	Residue
Fe-C	0.00	912	912.000	0.000
	0.05	883	887.042	-4.042
	0.11	856	860.541	-4.541
	0.16	838	841.253	-3.253
	0.22	821	821.299	-0.299
	0.27	809	807.147	1.853
	0.33	795	792.838	2.162
	0.38	786	782.254	3.146
	0.44	775	772.766	2.234
	0.49	766	765.544	0.456
	0.55	757	757.731	-0.731
	0.60	749	751.432	-2.432
	0.66	740	743.426	-3.426
	0.72	734	734.088	-0.088
	0.77	727	724.587	2.413
Fe-Mn	0.00	912	912.00	0.00
	0.49	893	893.14	-0.14
	0.98	875	874.61	0.39
	1.48	856	856.37	-0.37
	1.97	840	839.69	0.31
	2.46	825	824.96	0.04
Fe-Si	0.00	912	912.00	0.00
	0.25	927	927.82	-0.82
	0.51	946	946.09	-0.09
	0.76	967	967.16	-0.16
	1.02	996	995.81	0.19
	1.27	1033	1033.93	-0.93
	1.53	1090	1090.13	-0.13
Fe-Ni	0.00	912	912.00	0.00
	0.52	885	883.40	1.60
	1.05	860	860.95	-0.95
	1.58	845	844.15	0.85
	2.10	832	831.37	0.63
	2.63	820	819.53	0.47
Fe-Cr	0.00	912	912.00	0.00
	0.37	906	906.20	-0.20
	0.93	897	897.36	-0.36
	1.31	892	891.43	0.57
	1.86	883	883.26	-0.26
	2.24	878	878.17	-0.17
	2.80	872	872.05	-0.05

Table 3.1 continued

Ae_3 Temperature and Residue of Binary Systems

System	Composition (Wt%)	Expt. Ae_3 Temp. (^oC)	Calc. Ae_3 Temp. (^oC)	Residue
Fe-Mo	0.00	912	912.00	0.00
	0.43	922	923.08	-1.08
	0.86	937	937.15	-0.15
	1.28	956	955.00	1.00
	1.71	978	979.59	-1.59
	2.13	1013	1012.62	0.38
	2.55	1058	1058.17	-0.17
Fe-Cu	0.00	912	912.00	0.00
	0.22	906	906.20	-0.20
	0.44	901	900.92	0.08
	0.88	891	891.11	-0.11
	1.32	881	881.06	-0.06

calculated estimate of the dependent variable agrees with the actual value . It is defined as:

$$SE = \left[\frac{\Sigma (y_{expt} - y_{predicted})^2}{N} \right]^{1/2}$$

Residue of Error of Estimate: It is the difference in the experimental and predicted value of a dependent variable.

Residue = Expt. Value - Predicted Value

The Degree of Freedom: It is the excess amount of data points available to be used in the regression equation . As the degree of freedom increase , the accuracy of the results also increases. One hundred degrees of freedom and over is considered a respectable number for a regression system.

Sum of Squared Residuals: It is the sum of the square of the residues.

$$SSE = \sum_{i=1}^{n} e = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

Where y_i = observed value

$\hat{y}_i$ = predicted (estimated) value

3.3 Determination of Analytical Expression for Ae_3 Temperature:

In all the systems, the first coefficient A_o was fixed at 912^{o}C. Fifth order polynomial was tried in all the cases. The fifth degree term was found to be highly co-related with other terms and hence removed from the models in all the cases. Also the third degree terms were found to be highly co-related with other terms in all cases except, in Fe-Cu system where the fourth degree term was found to be related with other terms and hence these were removed from the models. We represent equations in the following form:

$$T_e = A_o + A_1 X + A_2 X^2 + A_3 X^3 + A_4 X^4$$

Where T_e is Ae_3 temperature in ^{o}C and X represent composition in weight percent.

Values of the various coefficients for different systems have been shown in Table 3.2.

Table 3.2

Coefficients in the Binary Regression Equations

Binary System	A_o	A_1	A_2	A_3	A_4
Fe-C	912	-526.0	528.0	0.0	272.00
Fe-Mn	912	-38.7	0.41	0.0	0.155
Fe-Si	912	61.0	8.37	0.0	11.9
Fe-Ni	912	-61.6	12.8	0.0	0.397
Fe-Cr	912	-15.6	-0.231	0.0	0.0901
Fe-Mo	912	22.8	6.71	0.0	1.05
Fe-Cu	912	-27.8	7.25	-2.99	0.0

3.4 Assessment of the Models:

3.4.1 Assessment Based on Statistical Parameters:

Values of the different statistical parameters give excellent indication of the goodness of the models.These are listed in Table 3.3 .

3.4.2 Assessment from the Plots:

Experimental Ae_3 temperature and predicted Ae_3 temperature can best be compared from the plots for the various systems. In plots shown in figures 3.1 to 3.7 , the circles represent the experimental Ae_3 temperature and the solid lines represent the corresponding models. It can be seen that there is excellent match between the two. Thus we see that models for these binary systems of Ae_3 temperature predict Ae_3 temperature fairly accurately.

3.4.3 Assessment Based on Predicted Temperature:

In general, the predicted temperature matches excellently with the observed Ae_3 temperature of the systems. This is seen from Table 3.1 which has both experimental and predicted values. In the case of Fe-C system , the maximum residue (absolute) is 4.54 The maximum residue (absolute) for other systems is not greater than 2.0 as can be seen from Table 3.3.

Table 3.3

Statistical Parameters of Calculated Ae_3 Temperatures of Binary Systems

System	SOSR	Mean of Residue	Max. Residue (absolute)	SE
Fe-C	94.85	-0.44	4.54	2.48
Fe-Mn	0.41	0.04	0.39	0.28
Fe-Si	1.62	-0.28	0.82	0.39
Fe-Ni	4.80	0.43	1.60	0.78
Fe-Cr	0.59	-0.07	0.57	0.28
Fe-Mo	4.89	-0.23	1.59	0.80
Fe-Cu	0.06	-0.06	0.20	0.10

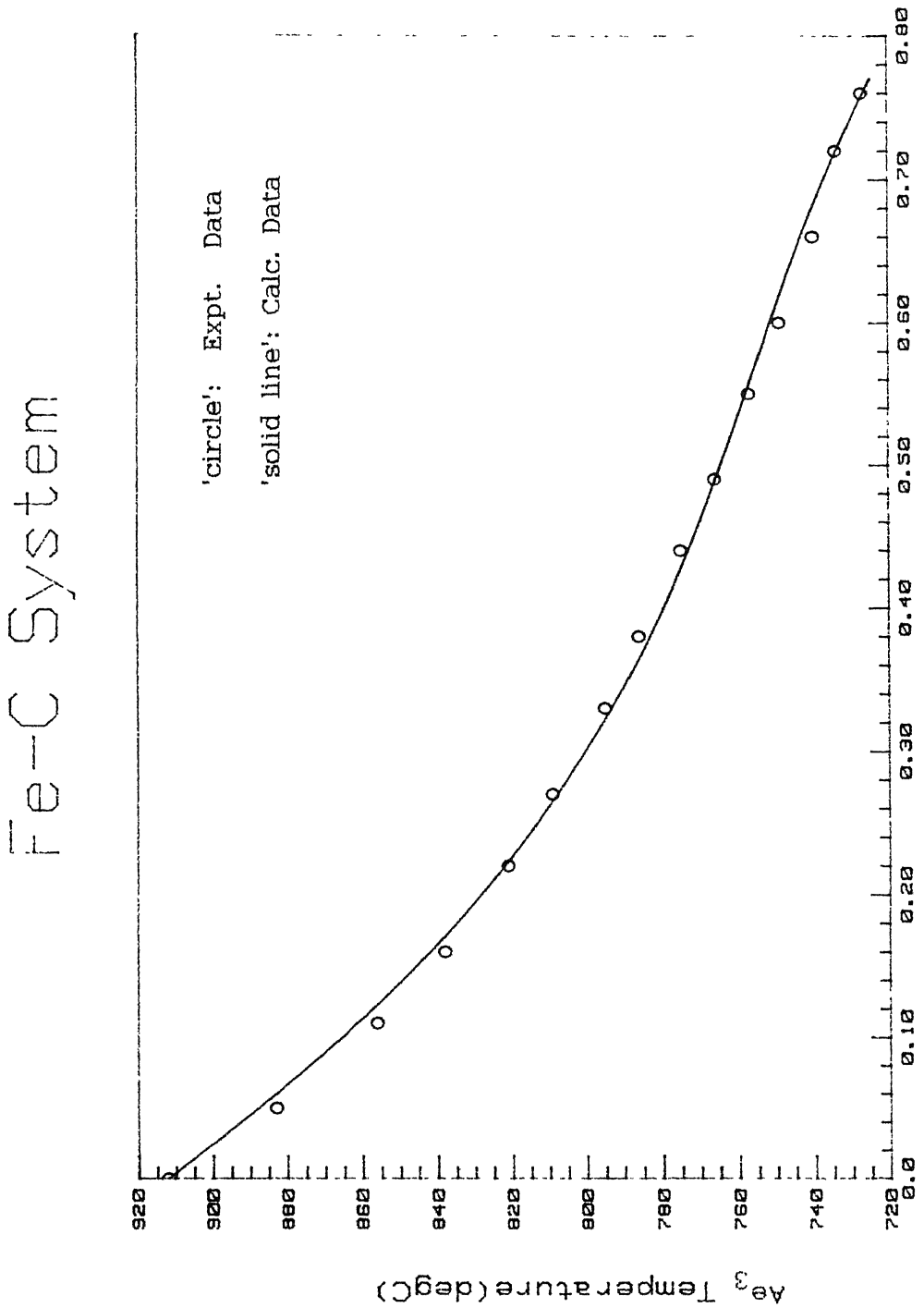

Fe-C System
'circle': Expt. Data
'solid line': Calc. Data
Ae_3 Temperature(degC)
Comp(Wt%)
920
900
880
860
840
820
800
780
760
740
720
0.0
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80

Figure 3.1

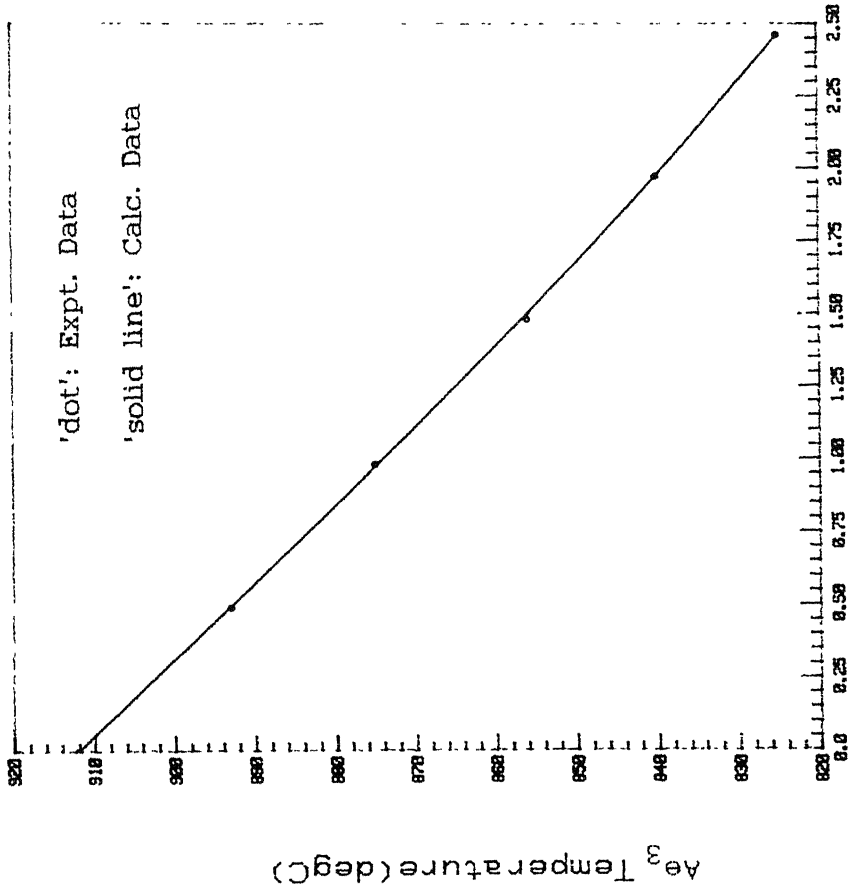


Figure 3.2

Fe-Mn System

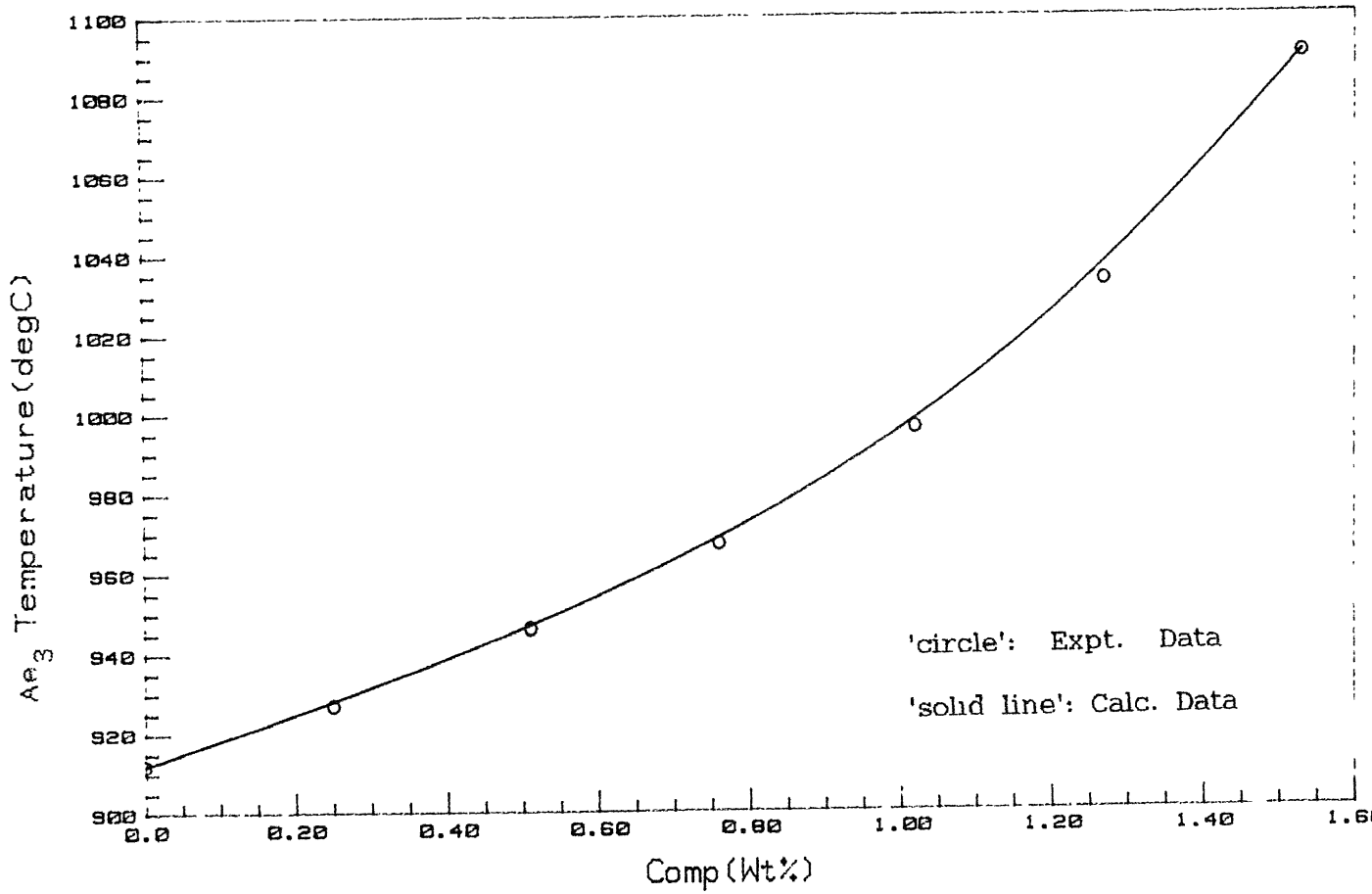

Fe-Si System
1100
1080
1060
1040
1020
1000
980
960
940
920
900
Ae3 Temperature(degC)
0.0
0.20
0.40
0.60
0.80
1.00
1.20
1.40
1.60
Comp(Wt%)
'circle': Expt. Data
'solid line': Calc. Data

Figure 3.3

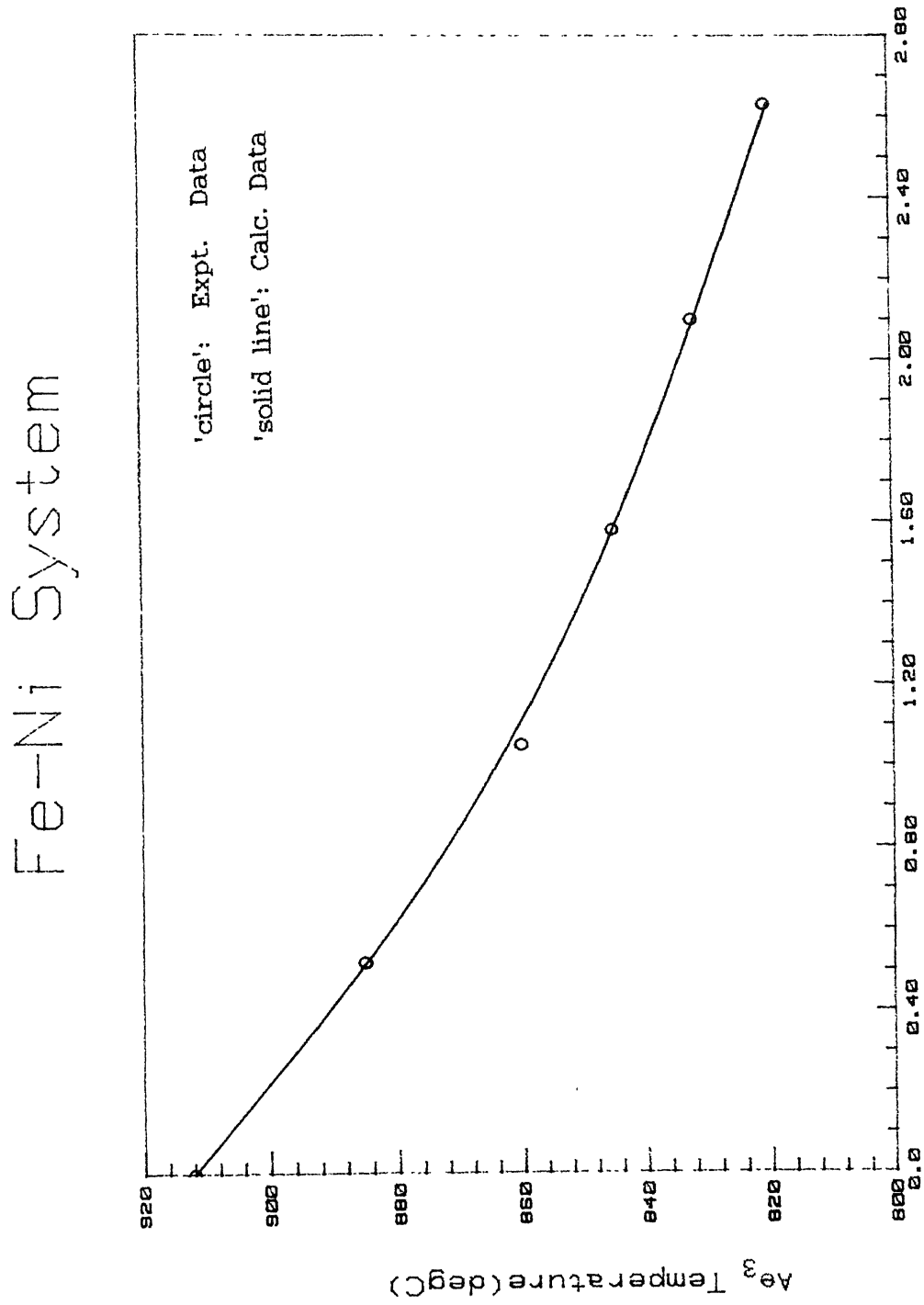

Fe-Ni System
'circle': Expt. Data
'solid line': Calc. Data
Ae3 Temperature(degC)
Comp(Wt%)
920
900
880
860
840
820
800
0.0
0.40
0.80
1.20
1.60
2.00
2.40
2.80

Figure 3.4

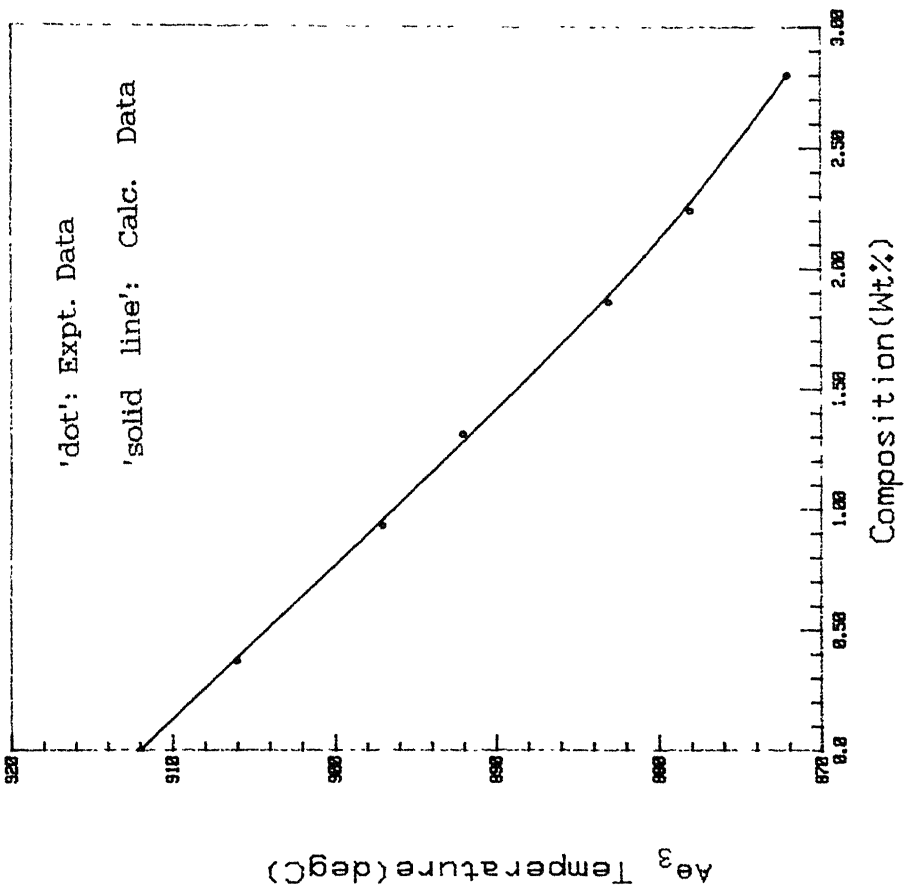


Figure 3.5
Fe-Cr System

Fe-Mo System

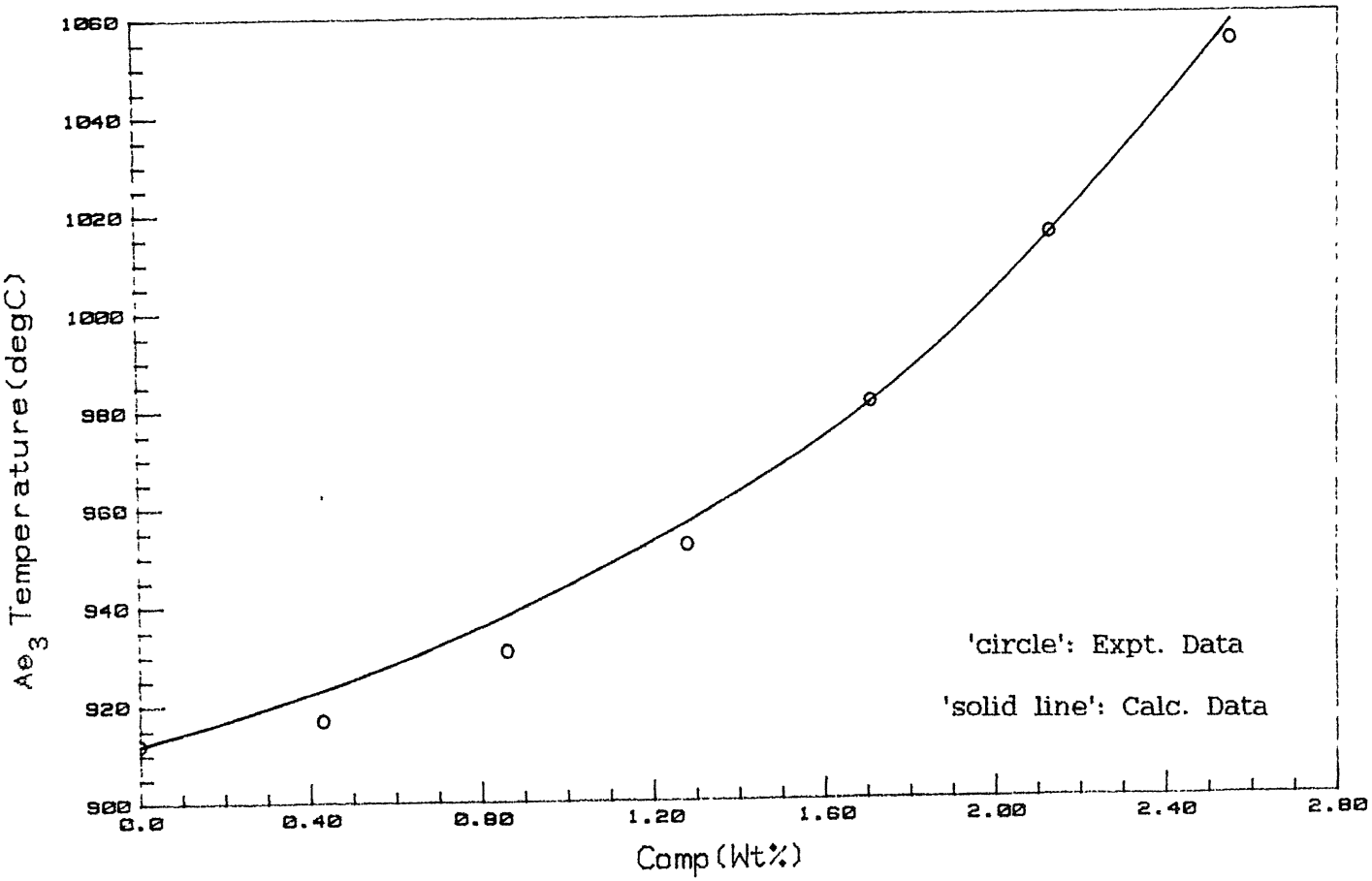
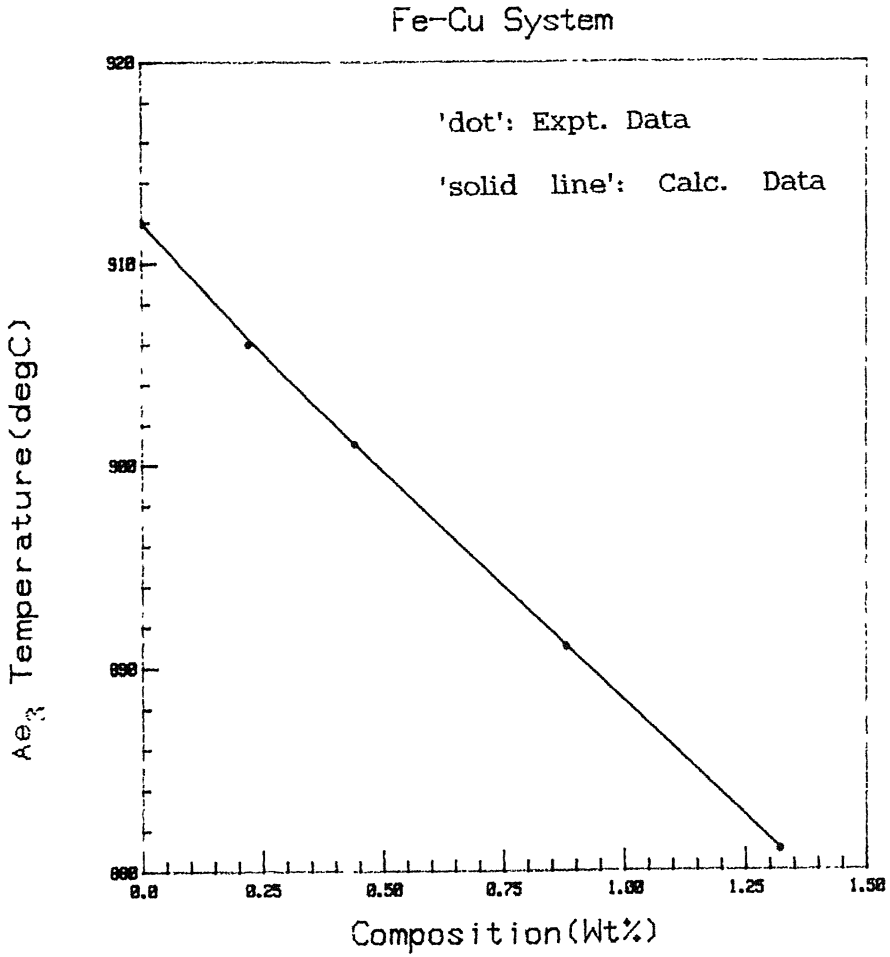


Figure 3.6

Figure 3.7


Fe-Cu System
'dot': Expt. Data
'solid line': Calc. Data
920
910
900
890
880
0.0
0.25
0.50
0.75
1.00
1.25
1.50
Ae3 Temperature(degC)
Composition(Wt%)

CHAPTER IV

Ae_3 TEMPERATURE OF MULTICOMPONENT STEELS

4.1 Introduction:

In this chapter , attempt is made to establish quantitative relationship between Ae_3 temperature and composition of multicomponent steels. As already pointed out in the literature review, there are many models available but their assumptions are unreasonable or they don't predict the result satisfactorily. In this chapter a mathematical model for multicomponent steels is developed.

4.2 Mathematical Formulation of the Model:

In low alloy steels austenite is essentially a dilute solution of several solutes in fcc iron. The Ae_3 temperature of alloys depends on the contents of the various solutes present in the alloys. Any functional relationship can be taken as polynomial relation. If we can determine the various parameters involved in the functional relation then our job is done.

Let's consider a steel containing various solutes 1 to n and solvent as 0. The Ae_3 temperature T_e can be expressed as the function of the various compositions in weight fraction as:

$$T_e = f(X_1, X_2, \ldots, X_i, \ldots, X_n)$$

Where X_i is the weight fraction of i^{th} alloying elements.

As already stated, any functional relationship can be expressed as polynomial series expansion provided we modify variables in such manner that the series converges. It is possible in our case, if the solution can be treated as dilute solution. The higher order terms can be neglected if the terms become smaller and smaller. Expressing

the relation as a polynomial:

$$T_e = \sum_{m_1} \cdots \sum_{m_i} \cdots \sum_{m_n} A_{m_1,\ldots,m_i,\ldots,m_n} X_1^{m_1} X_2^{m_2} \cdots X_i^{m_i} \cdots X_n^{m_n}$$

Here A's represent the coefficients of the series and each m stands for all positive inters including zero.

By the Taylor's series expansion around the composition where the weight fraction of the solvent tends to 1 , the coefficients of the series can be expressed as derivatives. Then:

$$A_{m_1,\ldots,m_i,\ldots,m_n} = \frac{1}{\sum_1^n m_i} \left[\frac{\partial^r T_e}{\partial X_1^{m_1} \cdots \partial X_i^{m_i} \cdots \partial X_n^{m_n}} \right]_{X_o \to 100}$$

Writing for convenience, the r^{th} order interaction coefficient as $A_{1m_1,\ldots,im_i,\ldots,nm_n}$, the Ae_3 temperature of the steel may be expressed as :

$$T_e = A_o + \sum_i A_i X_i + \sum_i A_{ii} X_i + \frac{1}{2} \sum_{\substack{i \\ i \neq k}} \sum_k A_{ik} X_i X_k + \cdots$$

Where i and k stand for alloying elements and A_o is the Ae_3 temperature of pure iron. The number of terms to be kept in the model depends on the accuracy we desire and the availability of the experimental data and also on the ease to handle the computation. If we retain only first order terms then the model reduces to:

$$T = A_o + A_1 X_1 + \ldots + A_i X_i + \ldots + A_n X_n$$

This is the equation equivalent to the Grange's [5] relation. If we desire terms containing up to second order then the model can be written as:

$$T_e = A_o + [\, A_1 X_1 + \ldots + A_i X_i + \ldots + A_n X_n] + [\, (A_{11} X_1^2 + A_{12} X_1 X_2 + \ldots + A_{1n} X_1 X_n) + A_{22} X_2^2 + A_{23} X_2 X_3 + \ldots + A_{2n} X_2 X_n) + \ldots \,]$$

Thus a model containing terms up to any order can be taken. The coefficients of the model are to be estimated on the basis of the available experimental data. Once that is done, the job is finished and then we can predict the Ae_3 temperature for any composition that approximate to dilute solution.

4.3 Assessment of the Available Data on Ae_3 Temperature:

Availability or selection of appropriate data is vital for determining coefficients of any model. Accuracy of the data is one important factor. Another important factor is that there should be sufficient number of experimental data available. It is also required that the data should be representative of the range in which we are going to predict on the basis of our model.

Unfortunately, a large part of the available data refers really to Ac_3 temperature (the Ac_3 temperature is the temperature at which the hypoeutectoid steel becomes fully austenite during continuous heating). The Ae_3 temperatures (the Ae_3 temperature is defined as the upper limit of austenite formation in hypoeutectoid steels, measured by continuously heating at some specified rate[5]) of only a limited number of steels are available. It is to be noted that the average of Ac_3 and Ar_3 temperature (Ar_3 temperature is defined as the highest temperature at which austenite to ferrite transformation takes place in hypoeutectoid steels when they are continuously cooled at some specified rate) will not give Ae_3 temperature as the

Table 4.1(a) Composition and Ae_3 temperature of Selected Steels when No Binary Coefficients are Fixed with $\alpha = 0.03$

Composition(Wt%)							Ae_3 temperature		Residue
C	Mn	Si	Ni	Cr	Mo	Cu	Expt.T	Calc.T	
.35	.37	.21	.00	.00	.00	.00	799.00	798.98	.02
.47	.57	.20	.00	.00	.00	.00	771.00	768.14	2.86
.63	.87	.22	.00	.00	.00	.00	735.00	738.66	-3.66
.35	1.85	.19	.00	.00	.00	.00	776.00	775.15	.85
.42	1.58	.30	.00	.00	.00	.00	771.00	769.68	1.32
.37	.68	.21	3.41	.00	.00	.00	732.00	732.13	-.13
.38	.72	.21	1.32	.49	.00	.00	755.00	767.78	-12.78
.35	.80	.24	.00	.00	.25	.00	796.00	799.11	-3.11
.48	.94	.16	.00	.00	.25	.00	762.00	765.70	-3.70
.33	.53	.27	.00	.90	.18	.00	796.00	806.00	-10.00
.37	.77	.15	.00	.98	.21	.00	785.00	788.32	-3.32
.44	.95	.23	.00	.93	.21	.00	773.00	776.71	-3.71
.43	.78	.24	1.79	.80	.33	.00	746.00	768.93	-22.93
.36	.63	.19	1.84	.00	.23	.00	757.00	764.13	-7.13
.42	.68	.16	.00	.93	.00	.00	773.00	776.37	-3.37
.30	.80	.29	.54	.56	.21	.00	787.00	803.63	-16.63
.50	.77	.22	.60	.51	.22	.00	751.00	764.16	-13.16
.44	.90	.25	.44	.54	.22	.00	779.00	774.99	4.01
.50	.77	.23	.60	.50	.21	.00	757.00	764.20	-7.20
.35	.37	.21	.06	.05	.00	.07	800.00	797.59	2.41
.54	.46	.20	.00	.00	.00	.00	756.00	756.19	-.19
.17	.92	.07	.04	.01	.01	.03	825.00	828.46	-3.46
.20	.81	.16	.00	.00	.00	.00	845.00	829.85	15.15
.50	.91	.13	.00	.00	.00	.00	766.00	756.34	9.66
.63	.87	.17	.02	.04	.00	.02	737.00	738.15	-1.15
.64	1.13	.09	.00	.00	.00	.00	744.00	733.06	10.94
.20	1.88	.30	.03	.04	.02	.04	816.00	816.00	.00
.35	1.85	.19	.01	.03	.00	.02	778.00	775.04	2.96
.43	1.58	.31	.01	.05	.01	.02	773.00	768.76	4.24
.61	.27	.21	.99	.04	.01	.04	745.00	742.59	2.41
.56	.26	.21	1.97	.04	.00	.02	732.00	738.27	-6.27
.59	.25	.21	3.90	.04	.01	.03	712.00	717.76	-5.76
.37	.68	.21	3.41	.05	.00	.07	734.00	732.19	1.81
.10	.52	.28	5.00	.07	.03	.00	774.00	779.48	-5.48
.40	.52	.28	5.00	.07	.03	.00	714.00	715.29	-1.29
.38	.37	.25	.07	.57	.00	.05	791.00	791.82	-.82
.42	.68	.16	.07	.93	.00	.05	782.00	775.23	6.77
.33	.45	.28	.06	1.97	.02	.04	807.00	800.98	6.02
.11	.38	.44	.15	5.46	.42	.00	839.00	837.60	1.40
.65	.68	.23	.02	.02	.10	.02	741.00	740.38	.62
.26	.87	.29	.03	.06	.26	.00	824.00	824.18	-.18
.35	.80	.24	.06	.06	.25	.00	802.00	798.21	3.79
.48	.94	.16	.04	.03	.25	.03	769.00	765.27	3.73
.68	.87	.26	.01	.03	.24	.03	744.00	738.05	5.95
.42	.20	.18	.00	.00	.21	.00	782.00	787.22	-5.22
.40	.42	.19	.06	.13	.53	.07	802.00	792.24	9.76
.36	.17	.16	.00	.00	.82	.00	800.00	805.36	-5.36
.22	.79	.24	.03	.08	.50	.02	814.00	838.48	-24.48
.40	.57	.03	3.49	.00	.01	.00	724.00	718.95	5.05
.41	.60	.03	3.51	.00	.21	.00	718.00	721.29	-3.29

Table 4.1(a) Continued

C	Mn	Si	Ni	Cr	Mo	Cu	Expt.T	Calc.T	Residue
.39	.56	.03	3.53	.00	.74	.00	718.00	727.14	-9.14
.50	.23	.53	.02	.05	.00	.02	780.00	778.25	1.75
.48	.57	.20	.06	.02	.01	.46	764.00	763.12	.88
.49	.54	.20	.06	.02	.01	1.49	755.00	755.19	-.19
.38	.72	.21	1.32	.49	.00	.02	754.00	767.69	-13.69
.11	.45	.18	3.33	1.52	.03	.00	782.00	772.75	9.25
.33	.53	.27	.00	.90	.18	.00	800.00	806.00	-6.00
.37	.77	.15	.04	.98	.21	.00	786.00	787.96	-1.96
.17	.57	.27	1.87	.45	.24	.00	810.00	810.62	-.62
.42	.78	.24	1.79	.80	.33	.00	748.00	770.10	-22.10
.15	.63	.28	1.90	.05	.24	.00	794.00	815.55	-21.55
.36	.63	.19	1.84	.06	.23	.00	755.00	764.69	-9.69
.16	.52	.27	3.36	.09	.19	.04	777.00	782.56	-5.56
.18	.79	.21	.52	.56	.19	.00	838.00	827.97	10.03
.30	.80	.29	.54	.55	.21	.00	792.00	803.66	-11.66
.59	.89	.24	.53	.64	.22	.00	745.00	755.07	-10.07
.44	.90	.25	.45	.54	.22	.00	775.00	774.91	.09
.24	.94	.47	.30	.34	.14	.00	844.00	831.05	12.95
.10	1.63	.21	.00	.00	.41	.00	864.00	850.68	13.32
.63	.87	.17	.02	.04	.00	.02	736.00	738.15	-2.15
.14	.81	.34	1.81	.49	.27	.00	810.00	823.43	-13.43
.16	.60	.27	1.92	.06	.27	.00	800.00	812.49	-12.49
.18	.57	.24	.31	.31	.15	.00	850.00	840.32	9.68
.43	1.02	.26	.31	.48	.13	.00	770.00	775.24	-5.24
.22	.76	.20	.57	.51	.20	.00	832.00	817.13	14.87
.45	.89	.31	.59	.66	.12	.00	773.00	773.01	-.01
.50	.77	.23	.60	.50	.21	.00	755.00	764.20	-9.20
.19	.77	.24	.42	.40	.12	.00	827.00	829.63	-2.63
.46	.79	.38	.91	.77	.18	.00	782.00	773.33	8.67
.18	.67	.17	1.07	.00	.00	.00	824.00	814.82	9.18
.19	.75	.18	1.04	.00	.00	.00	823.00	812.56	10.44
.17	1.65	.16	1.07	.00	.00	.00	800.00	812.12	-12.12
.21	.75	.18	1.08	.48	.00	.00	811.00	803.46	7.54
.21	.78	.19	1.09	.99	.00	.00	800.00	800.52	-.52
.22	.77	.19	1.08	1.91	.00	.00	786.00	793.89	-7.89
.18	.65	.12	1.09	.00	.26	.00	811.00	816.38	-5.38
.21	.70	.15	1.08	.00	.49	.00	823.00	814.05	8.95
.18	.75	.71	1.07	.00	.00	.00	855.00	852.00	3.00
.27	1.12	.00	.00	.00	.00	.00	813.00	794.63	18.37
.37	.77	.15	.04	.98	.21	.00	787.00	787.96	-.96
.22	.79	.24	.03	.08	.50	.02	812.00	838.48	-26.48
.11	.00	1.83	.00	.00	.00	.00	990.00	1013.78	-23.78
.40	.00	1.73	.00	.00	.00	.00	860.00	857.43	2.57
.13	.00	.00	.00	2.99	.00	.00	817.00	827.17	-10.17
.41	.00	.00	.00	2.99	.00	.00	787.00	780.96	6.04
.13	.00	.00	.00	.00	.39	.00	875.00	869.67	5.33
.40	.00	.00	.00	.00	.38	.00	795.00	789.72	5.28
.12	3.08	.00	.00	.00	.00	.00	765.00	779.41	-14.41
.37	3.14	.00	.00	.00	.00	.00	725.00	743.27	-18.27
.11	.00	.00	3.28	.00	.00	.00	775.00	770.36	4.64
.37	.00	.00	3.04	.00	.00	.00	733.00	739.90	-6.90

Table 4.1(a) Continued

C	Mn	Si	Ni	Cr	Mo	Cu	Expt.T	Calc.T	Residue
.11	.00	.00	.00	.00	1.95	.00	902.00	899.76	2.24
.46	2.94	.00	.00	.00	.00	.00	730.00	734.67	-4.67
.22	5.01	.00	.00	.00	.00	.00	730.00	722.96	7.04
.30	2.43	.00	.00	.00	.00	.00	762.00	764.79	-2.79
.00	1.80	.00	.00	2.90	.00	.00	800.00	801.40	-1.40
.00	1.70	.00	.00	2.80	.00	.00	800.00	806.11	-6.11
.00	2.00	.00	.00	3.60	.00	.00	800.00	787.19	12.81
.00	1.60	.00	.00	2.50	.00	.00	800.00	813.60	-13.60
.00	3.30	.00	.00	5.50	.00	.00	750.00	752.63	-2.63
.00	3.20	.00	.00	4.40	.00	.00	750.00	747.35	2.65
.16	.00	.00	.00	2.40	.00	.00	829.00	826.34	2.66
.17	.00	.00	.00	3.16	.00	.00	820.00	816.54	3.46
.14	.00	.00	.00	3.83	.00	.00	807.00	815.64	-8.64
.15	.00	.00	.00	4.15	.00	.00	804.00	810.35	-6.35
.34	1.06	.20	.75	.23	.02	.00	800.00	782.12	17.88
.51	.23	.17	5.26	.04	.01	.00	710.00	705.70	4.30
.35	.65	.13	1.27	.55	.00	.00	790.00	769.93	20.07
.33	.57	.23	3.26	.85	.09	.00	750.00	753.41	-3.41
.29	.21	.06	3.25	1.45	.00	.00	733.00	738.39	-5.39
.35	.44	.14	4.23	1.43	.13	.00	755.00	759.35	-4.35
.32	.56	.27	2.37	.74	.51	.00	780.00	787.77	-7.77
.33	.51	.00	.82	2.32	.36	.00	792.00	785.60	6.40
.38	.56	.15	2.42	.74	.46	.00	770.00	772.47	-2.47
.40	1.38	.24	.74	.53	.16	.00	785.00	776.95	8.05
.41	.48	.09	1.75	.17	.22	.00	775.00	756.49	18.51
.44	.58	.23	1.40	1.26	.11	.00	775.00	767.56	7.44
.32	.51	.19	3.02	1.37	.48	.00	790.00	808.51	-18.51
.38	1.08	.70	.34	.40	.11	.00	804.00	803.24	.76
.12	.45	.40	.31	.62	.00	.26	879.00	879.78	-.78
.00	.00	.00	.00	.00	.00	.00	912.00	912.00	.00
.05	.00	.00	.00	.00	.00	.00	883.00	891.47	-8.47
.11	.00	.00	.00	.00	.00	.00	856.00	868.47	-12.47
.16	.00	.00	.00	.00	.00	.00	838.00	850.66	-12.66
.22	.00	.00	.00	.00	.00	.00	821.00	830.92	-9.92
.27	.00	.00	.00	.00	.00	.00	809.00	815.84	-6.84
.33	.00	.00	.00	.00	.00	.00	795.00	799.37	-4.37
.38	.00	.00	.00	.00	.00	.00	786.00	787.01	-1.01
.44	.00	.00	.00	.00	.00	.00	775.00	773.82	1.18
.49	.00	.00	.00	.00	.00	.00	766.00	764.18	1.82
.55	.00	.00	.00	.00	.00	.00	757.00	754.25	2.75
.60	.00	.00	.00	.00	.00	.00	749.00	747.34	1.66
.66	.00	.00	.00	.00	.00	.00	740.00	740.67	-.67
.72	.00	.00	.00	.00	.00	.00	734.00	735.80	-1.80
.77	.00	.00	.00	.00	.00	.00	727.00	733.09	-6.09
.00	.49	.00	.00	.00	.00	.00	893.00	893.95	-.95
.00	.98	.00	.00	.00	.00	.00	875.00	875.91	-.91
.00	1.48	.00	.00	.00	.00	.00	856.00	857.49	-1.49
.00	1.97	.00	.00	.00	.00	.00	840.00	839.44	.56
.00	2.46	.00	.00	.00	.00	.00	825.00	821.40	3.60
.00	.00	.25	.00	.00	.00	.00	927.00	935.27	-8.27
.00	.00	.51	.00	.00	.00	.00	946.00	959.47	-13.47
.00	.00	.76	.00	.00	.00	.00	967.00	982.74	-15.74

Table 4.1(a) Continued

C	Mn	Si	Ni	Cr	Mo	Cu	Expt.T	Calc.T	Residue
.00	.00	1.02	.00	.00	.00	.00	996.00	1006.94	-10.94
.00	.00	1.27	.00	.00	.00	.00	1033.00	1030.21	2.79
.00	.00	1.53	.00	.00	.00	.00	1090.00	1054.41	35.59
.00	.00	.00	.52	.00	.00	.00	885.00	893.45	-8.45
.00	.00	.00	1.05	.00	.00	.00	860.00	874.54	-14.54
.00	.00	.00	1.58	.00	.00	.00	845.00	855.63	-10.63
.00	.00	.00	2.10	.00	.00	.00	832.00	837.07	-5.07
.00	.00	.00	2.63	.00	.00	.00	820.00	818.16	1.84
.00	.00	.00	.00	.37	.00	.00	906.00	905.79	.21
.00	.00	.00	.00	.93	.00	.00	897.00	896.39	.61
.00	.00	.00	.00	1.31	.00	.00	892.00	890.02	1.98
.00	.00	.00	.00	1.86	.00	.00	883.00	880.79	2.21
.00	.00	.00	.00	2.24	.00	.00	878.00	874.41	3.59
.00	.00	.00	.00	2.80	.00	.00	872.00	865.02	6.98
.00	.00	.00	.00	.00	.43	.00	922.00	921.97	.03
.00	.00	.00	.00	.00	.86	.00	937.00	934.57	2.43
.00	.00	.00	.00	.00	1.28	.00	956.00	951.92	4.08
.00	.00	.00	.00	.00	1.71	.00	978.00	977.43	.57
.00	.00	.00	.00	.00	2.13	.00	1013.00	1012.40	.60
.00	.00	.00	.00	.00	2.55	.00	1058.00	1059.78	-1.78
.00	.00	.00	.00	.00	.00	.22	906.00	906.81	-.81
.00	.00	.00	.00	.00	.00	.44	901.00	901.61	-.61
.00	.00	.00	.00	.00	.00	.88	891.00	891.22	-.22
.00	.00	.00	.00	.00	.00	1.32	881.00	880.83	.17

Table 4.1(b) Composition and Ae_3 temperatures of Selected Steels when No Binary Coefficients are Fixed $\alpha = 0.01$

Composition(Wt%)							Ae_3 temperature		Residue
C	Mn	Si	Ni	Cr	Mo	Cu	Expt.T	Calc.T	
.35	.37	.21	.00	.00	.00	.00	799.00	800.27	-1.27
.47	.57	.20	.00	.00	.00	.00	771.00	769.29	1.71
.63	.87	.22	.00	.00	.00	.00	735.00	738.91	-3.91
.35	1.85	.19	.00	.00	.00	.00	776.00	775.88	.12
.42	1.58	.30	.00	.00	.00	.00	771.00	770.17	.83
.37	.68	.21	3.41	.00	.00	.00	732.00	734.12	-2.12
.38	.72	.21	1.32	.49	.00	.00	755.00	767.16	-12.16
.35	.80	.24	.00	.00	.25	.00	796.00	799.50	-3.50
.48	.94	.16	.00	.00	.25	.00	762.00	765.77	-3.77
.33	.53	.27	.00	.90	.18	.00	796.00	806.20	-10.20
.37	.77	.15	.00	.98	.21	.00	785.00	788.23	-3.23
.44	.95	.23	.00	.93	.21	.00	773.00	776.29	-3.29
.43	.78	.24	1.79	.80	.33	.00	746.00	768.30	-22.30
.36	.63	.19	1.84	.00	.23	.00	757.00	760.82	-3.82
.42	.68	.16	.00	.93	.00	.00	773.00	776.84	-3.84
.30	.80	.29	.54	.56	.21	.00	787.00	802.13	-15.13
.50	.77	.22	.60	.51	.22	.00	751.00	761.83	-10.83
.44	.90	.25	.44	.54	.22	.00	779.00	772.92	6.08
.50	.77	.23	.60	.50	.21	.00	757.00	761.87	-4.87
.35	.37	.21	.06	.05	.00	.07	800.00	797.85	2.15
.54	.46	.20	.00	.00	.00	.00	756.00	757.36	-1.36
.17	.92	.07	.04	.01	.01	.03	825.00	829.35	-4.35
.20	.81	.16	.00	.00	.00	.00	845.00	830.93	14.07
.50	.91	.13	.00	.00	.00	.00	766.00	757.12	8.88
.63	.87	.17	.02	.04	.00	.02	737.00	738.03	-1.03
.64	1.13	.09	.00	.00	.00	.00	744.00	732.86	11.14
.20	1.88	.30	.03	.04	.02	.04	816.00	815.04	.96
.35	1.85	.19	.01	.03	.00	.02	778.00	775.29	2.71
.43	1.58	.31	.01	.05	.01	.02	773.00	768.22	4.78
.61	.27	.21	.99	.04	.01	.04	745.00	737.15	7.85
.56	.26	.21	1.97	.04	.00	.02	732.00	731.21	.79
.59	.25	.21	3.90	.04	.01	.03	712.00	711.23	.77
.37	.68	.21	3.41	.05	.00	.07	734.00	734.43	-.43
.10	.52	.28	5.00	.07	.03	.00	774.00	761.81	12.19
.40	.52	.28	5.00	.07	.03	.00	714.00	726.51	-12.51
.38	.37	.25	.07	.57	.00	.05	791.00	791.62	-.62
.42	.68	.16	.07	.93	.00	.05	782.00	775.44	6.56
.33	.45	.28	.06	1.97	.02	.04	807.00	800.18	6.82
.11	.38	.44	.15	5.46	.42	.00	839.00	836.50	2.50
.65	.68	.23	.02	.02	.10	.02	741.00	740.04	.96
.26	.87	.29	.03	.06	.26	.00	824.00	824.32	-.32
.35	.80	.24	.06	.06	.25	.00	802.00	798.11	3.89
.48	.94	.16	.04	.03	.25	.03	769.00	764.76	4.24
.68	.87	.26	.01	.03	.24	.03	744.00	736.51	7.49
.42	.20	.18	.00	.00	.21	.00	782.00	788.06	-6.06
.40	.42	.19	.06	.13	.53	.07	802.00	791.23	10.77
.36	.17	.16	.00	.00	.82	.00	800.00	804.76	-4.76
.22	.79	.24	.03	.08	.50	.02	814.00	837.70	-23.70
.40	.57	.03	3.49	.00	.01	.00	724.00	721.86	2.14
.41	.60	.03	3.51	.00	.21	.00	718.00	724.70	-6.70
.39	.56	.03	3.53	.00	.74	.00	718.00	728.65	-10.65

Table 4.1(b) Continued

C	Mn	Si	Ni	Cr	Mo	Cu	Expt.T	Calc.T	Residue
.30	2.43	.00	.00	.00	.00	.00	762.00	765.62	-3.62
.00	1.80	.00	.00	2.90	.00	.00	800.00	802.30	-2.30
.00	1.70	.00	.00	2.80	.00	.00	800.00	806.98	-6.98
.00	2.00	.00	.00	3.60	.00	.00	800.00	787.99	12.01
.00	1.60	.00	.00	2.50	.00	.00	800.00	814.46	-14.46
.00	3.30	.00	.00	5.50	.00	.00	750.00	752.09	-2.09
.00	3.20	.00	.00	4.40	.00	.00	750.00	748.01	1.99
.16	.00	.00	.00	2.40	.00	.00	829.00	826.54	2.46
.17	.00	.00	.00	3.16	.00	.00	820.00	816.54	3.46
.14	.00	.00	.00	3.83	.00	.00	807.00	815.54	-8.54
.15	.00	.00	.00	4.15	.00	.00	804.00	810.15	-6.15
.34	1.06	.20	.75	.23	.02	.00	800.00	777.19	22.81
.51	.23	.17	5.26	.04	.01	.00	710.00	701.51	8.49
.35	.65	.13	1.27	.55	.00	.00	790.00	769.69	20.31
.33	.57	.23	3.26	.85	.09	.00	750.00	758.21	-8.21
.29	.21	.06	3.25	1.45	.00	.00	733.00	741.47	-8.47
.35	.44	.14	4.23	1.43	.13	.00	755.00	752.75	2.25
.32	.56	.27	2.37	.74	.51	.00	780.00	775.07	4.93
.33	.51	.00	.82	2.32	.36	.00	792.00	783.92	8.08
.38	.56	.15	2.42	.74	.46	.00	770.00	761.42	8.58
.40	1.38	.24	.74	.53	.16	.00	785.00	770.65	14.35
.41	.48	.09	1.75	.17	.22	.00	775.00	753.03	21.97
.44	.58	.23	1.40	1.26	.11	.00	775.00	770.84	4.16
.32	.51	.19	3.02	1.37	.48	.00	790.00	769.95	20.05
.38	1.08	.70	.34	.40	.11	.00	804.00	801.11	2.89
.12	.45	.40	.31	.62	.00	.26	879.00	864.51	14.49
.00	.00	.00	.00	.00	.00	.00	912.00	912.00	.00
.05	.00	.00	.00	.00	.00	.00	883.00	891.73	-8.73
.11	.00	.00	.00	.00	.00	.00	856.00	869.02	-13.02
.16	.00	.00	.00	.00	.00	.00	838.00	851.44	-13.44
.22	.00	.00	.00	.00	.00	.00	821.00	831.95	-10.95
.27	.00	.00	.00	.00	.00	.00	809.00	817.04	-8.04
.33	.00	.00	.00	.00	.00	.00	795.00	800.76	-5.76
.38	.00	.00	.00	.00	.00	.00	786.00	788.54	-2.54
.44	.00	.00	.00	.00	.00	.00	775.00	775.48	-.48
.49	.00	.00	.00	.00	.00	.00	766.00	765.94	.06
.55	.00	.00	.00	.00	.00	.00	757.00	756.09	.91
.60	.00	.00	.00	.00	.00	.00	749.00	749.23	-.23
.66	.00	.00	.00	.00	.00	.00	740.00	742.61	-2.61
.72	.00	.00	.00	.00	.00	.00	734.00	737.73	-3.73
.77	.00	.00	.00	.00	.00	.00	727.00	735.01	-8.01
.00	.49	.00	.00	.00	.00	.00	893.00	894.22	-1.22
.00	.98	.00	.00	.00	.00	.00	875.00	876.45	-1.45
.00	1.48	.00	.00	.00	.00	.00	856.00	858.31	-2.31
.00	1.97	.00	.00	.00	.00	.00	840.00	840.53	-.53
.00	2.46	.00	.00	.00	.00	.00	825.00	822.75	2.25
.00	.00	.25	.00	.00	.00	.00	927.00	935.40	-8.40
.00	.00	.51	.00	.00	.00	.00	946.00	959.74	-13.74
.00	.00	.76	.00	.00	.00	.00	967.00	983.14	-16.14
.00	.00	1.02	.00	.00	.00	.00	996.00	1007.47	-11.47
.00	.00	1.27	.00	.00	.00	.00	1033.00	1030.87	2.13
.00	.00	1.53	.00	.00	.00	.00	1090.00	1055.21	34.79
.00	.00	.00	.52	.00	.00	.00	885.00	894.56	-9.56
.00	.00	.00	1.05	.00	.00	.00	860.00	876.79	-16.79

Table 4.1(b) Continued

C	Mn	Si	Ni	Cr	Mo	Cu	Expt.T	Calc.T	Residu
.50	.23	.53	.02	.05	.00	.02	780.00	777.16	2.84
.48	.57	.20	.06	.02	.01	.46	764.00	759.74	4.26
.49	.54	.20	.06	.02	.01	1.49	755.00	742.93	12.07
.38	.72	.21	1.32	.49	.00	.02	754.00	766.86	-12.86
.11	.45	.18	3.33	1.52	.03	.00	782.00	770.50	11.50
.33	.53	.27	.00	.90	.18	.00	800.00	806.20	-6.20
.37	.77	.15	.04	.98	.21	.00	786.00	787.79	-1.79
.17	.57	.27	1.87	.45	.24	.00	810.00	807.00	3.00
.42	.78	.24	1.79	.80	.33	.00	748.00	769.20	-21.20
.15	.63	.28	1.90	.05	.24	.00	794.00	812.61	-18.61
.36	.63	.19	1.84	.06	.23	.00	755.00	761.52	-6.52
.16	.52	.27	3.36	.09	.19	.04	777.00	777.24	-.24
.18	.79	.21	.52	.56	.19	.00	838.00	826.56	11.44
.30	.80	.29	.54	.55	.21	.00	792.00	802.14	-10.14
.59	.89	.24	.53	.64	.22	.00	745.00	752.73	-7.73
.44	.90	.25	.45	.54	.22	.00	775.00	772.82	2.18
.24	.94	.47	.30	.34	.14	.00	844.00	829.92	14.08
.10	1.63	.21	.00	.00	.41	.00	864.00	850.70	13.30
.63	.87	.17	.02	.04	.00	.02	736.00	738.03	-2.03
.14	.81	.34	1.81	.49	.27	.00	810.00	816.74	-6.74
.16	.60	.27	1.92	.06	.27	.00	800.00	809.85	-9.85
.18	.57	.24	.31	.31	.15	.00	850.00	840.11	9.89
.43	1.02	.26	.31	.48	.13	.00	770.00	773.28	-3.28
.22	.76	.20	.57	.51	.20	.00	832.00	815.60	16.40
.45	.89	.31	.59	.66	.12	.00	773.00	771.47	1.53
.50	.77	.23	.60	.50	.21	.00	755.00	761.87	-6.87
.19	.77	.24	.42	.40	.12	.00	827.00	828.66	-1.66
.46	.79	.38	.91	.77	.18	.00	782.00	772.87	9.13
.18	.67	.17	1.07	.00	.00	.00	824.00	812.35	11.65
.19	.75	.18	1.04	.00	.00	.00	823.00	809.29	13.71
.17	1.65	.16	1.07	.00	.00	.00	800.00	791.18	8.82
.21	.75	.18	1.08	.48	.00	.00	811.00	801.76	9.24
.21	.78	.19	1.09	.99	.00	.00	800.00	800.54	-.54
.22	.77	.19	1.08	1.91	.00	.00	786.00	797.74	-11.74
.18	.65	.12	1.09	.00	.26	.00	811.00	813.64	-2.64
.21	.70	.15	1.08	.00	.49	.00	823.00	810.61	12.39
.18	.75	.71	1.07	.00	.00	.00	855.00	848.80	6.20
.27	1.12	.00	.00	.00	.00	.00	813.00	795.73	17.27
.37	.77	.15	.04	.98	.21	.00	787.00	787.79	-.79
.22	.79	.24	.03	.08	.50	.02	812.00	837.70	-25.70
.11	.00	1.83	.00	.00	.00	.00	990.00	1014.95	-24.95
.40	.00	1.73	.00	.00	.00	.00	860.00	858.73	1.27
.13	.00	.00	.00	2.99	.00	.00	817.00	827.25	-10.25
.41	.00	.00	.00	2.99	.00	.00	787.00	780.50	6.50
.13	.00	.00	.00	.00	.39	.00	875.00	869.20	5.80
.40	.00	.00	.00	.00	.38	.00	795.00	790.22	4.78
.12	3.08	.00	.00	.00	.00	.00	765.00	781.04	-16.04
.37	3.14	.00	.00	.00	.00	.00	725.00	743.33	-18.33
.11	.00	.00	3.28	.00	.00	.00	775.00	771.98	3.02
.37	.00	.00	3.04	.00	.00	.00	733.00	729.27	3.73
.11	.00	.00	.00	.00	1.95	.00	902.00	899.26	2.74
.46	2.94	.00	.00	.00	.00	.00	730.00	733.85	-3.85
.22	5.01	.00	.00	.00	.00	.00	730.00	724.35	5.65

Table 4.1(b) Continued

C	Mn	Si	Ni	Cr	Mo	Cu	Expt.T	Calc.T	Residue
.00	.00	.00	1.58	.00	.00	.00	845.00	859.02	-14.02
.00	.00	.00	2.10	.00	.00	.00	832.00	841.59	-9.59
.00	.00	.00	2.63	.00	.00	.00	820.00	823.82	-3.82
.00	.00	.00	.00	.37	.00	.00	906.00	905.81	.19
.00	.00	.00	.00	.93	.00	.00	897.00	896.43	.57
.00	.00	.00	.00	1.31	.00	.00	892.00	890.07	1.93
.00	.00	.00	.00	1.86	.00	.00	883.00	880.86	2.14
.00	.00	.00	.00	2.24	.00	.00	878.00	874.50	3.50
.00	.00	.00	.00	2.80	.00	.00	872.00	865.13	6.87
.00	.00	.00	.00	.00	.43	.00	922.00	920.74	1.26
.00	.00	.00	.00	.00	.86	.00	937.00	932.37	4.63
.00	.00	.00	.00	.00	1.28	.00	956.00	949.30	6.70
.00	.00	.00	.00	.00	1.71	.00	978.00	975.17	2.83
.00	.00	.00	.00	.00	2.13	.00	1013.00	1011.53	1.47
.00	.00	.00	.00	.00	2.55	.00	1058.00	1061.58	-3.58
.00	.00	.00	.00	.00	.00	.22	906.00	908.74	-2.74
.00	.00	.00	.00	.00	.00	.44	901.00	905.49	-4.49
.00	.00	.00	.00	.00	.00	.88	891.00	898.98	-7.98
.00	.00	.00	.00	.00	.00	1.32	881.00	892.46	-11.46

Table 4.1(c) Composition and Ae_3 temperatures of Selected Steels when Binary Si Coefficients are Fixed with α = 0.005

Composition(Wt%)							Ae_3 temperature		Residue
C	Mn	Si	Ni	Cr	Mo	Cu	Expt.T	Calc.T	
.35	.37	.21	.00	.00	.00	.00	799.00	798.86	.14
.47	.57	.20	.00	.00	.00	.00	771.00	769.58	1.42
.63	.87	.22	.00	.00	.00	.00	735.00	741.97	-6.97
.35	1.85	.19	.00	.00	.00	.00	776.00	779.61	3.61
.42	1.58	.30	.00	.00	.00	.00	771.00	775.90	4.90
.37	.68	.21	3.41	.00	.00	.00	732.00	741.12	9.12
.38	.72	.21	1.32	.49	.00	.00	755.00	769.13	14.13
.35	.80	.24	.00	.00	.25	.00	796.00	798.14	2.14
.48	.94	.16	.00	.00	.25	.00	762.00	766.41	4.41
.33	.53	.27	.00	.90	.18	.00	796.00	803.31	7.31
.37	.77	.15	.00	.98	.21	.00	785.00	787.53	2.53
.44	.95	.23	.00	.93	.21	.00	773.00	777.07	-4.07
.43	.78	.24	1.79	.80	.33	.00	746.00	762.60	16.60
.36	.63	.19	1.84	.00	.23	.00	757.00	766.79	9.79
.42	.68	.16	.00	.93	.00	.00	773.00	778.66	5.66
.30	.80	.29	.54	.56	.21	.00	787.00	801.24	14.24
.50	.77	.22	.60	.51	.22	.00	751.00	760.69	9.69
.44	.90	.25	.44	.51	.22	.00	779.00	772.69	6.31
.50	.77	.23	.60	.50	.21	.00	757.00	760.83	3.83
.35	.37	.21	.06	.05	.00	.07	800.00	796.28	3.72
.54	.46	.20	.00	.00	.00	.00	756.00	755.39	.61
.17	.92	.07	.04	.01	.01	.03	825.00	830.96	-5.96
.20	.81	.16	.00	.00	.00	.00	845.00	831.40	13.60
.50	.91	.13	.00	.00	.00	.00	766.00	761.64	4.36
.63	.87	.17	.02	.04	.00	.02	737.00	741.03	-4.03
.64	1.13	.09	.00	.00	.00	.00	744.00	741.69	2.31
.20	1.88	.30	.03	.04	.02	.04	816.00	815.71	.29
.35	1.85	.19	.01	.03	.00	.02	778.00	778.94	-.94
.43	1.58	.31	.01	.05	.01	.02	773.00	774.07	-1.07
.61	.27	.21	.99	.04	.01	.04	745.00	733.50	11.50
.56	.26	.21	1.97	.04	.00	.02	732.00	733.08	-1.08
.59	.25	.21	3.90	.04	.01	.03	712.00	714.27	2.27
.37	.68	.21	3.41	.05	.00	.07	734.00	739.59	-5.59
.10	.52	.28	5.00	.07	.03	.00	774.00	766.38	7.62
.40	.52	.28	5.00	.07	.03	.00	714.00	714.40	-.40
.38	.37	.25	.07	.57	.00	.05	791.00	790.54	.46
.42	.68	.16	.07	.93	.00	.05	782.00	778.35	3.65
.33	.45	.28	.06	1.97	.02	.04	807.00	799.52	7.48
.11	.38	.44	.15	5.46	.47	.00	839.00	840.85	-1.85
.65	.68	.23	.02	.02	.10	.02	741.00	738.85	2.15
.26	.87	.29	.03	.06	.26	.00	824.00	821.80	2.20
.35	.80	.24	.06	.06	.25	.00	802.00	797.03	4.97
.48	.94	.16	.04	.03	.25	.03	769.00	765.40	3.60
.68	.87	.26	.01	.03	.24	.03	744.00	737.18	6.82
.42	.20	.18	.00	.00	.21	.00	782.00	781.07	.93
.40	.42	.19	.06	.13	.53	.07	802.00	786.05	15.95
.36	.17	.16	.00	.00	.82	.00	800.00	798.55	1.45
.22	.79	.24	.03	.08	.50	.02	814.00	833.39	-19.39
.40	.57	.03	3.49	.00	.01	.00	774.00	774.91	-.91
.41	.60	.03	3.51	.00	.21	.00	718.00	725.01	-7.01
.39	.56	.03	3.53	.00	.24	.00	718.00	727.74	-9.74

Table 4.1(c) Continued

C	Mn	Si	Ni	Cr	Mo	Cu	Expt.T	Calc.T	Residue
.50	.23	.53	.02	.05	.00	.02	780.00	790.73	-10.73
.48	.57	.20	.06	.02	.01	.46	764.00	758.99	5.01
.49	.54	.20	.06	.02	.01	1.49	755.00	757.11	-2.11
.38	.72	.21	1.32	.49	.00	.02	754.00	768.83	-14.83
.11	.45	.18	3.33	1.52	.03	.00	782.00	770.46	11.54
.33	.53	.27	.00	.90	.18	.00	800.00	803.31	-3.31
.37	.77	.15	.04	.98	.21	.00	786.00	787.04	-1.04
.17	.57	.27	1.87	.45	.24	.00	810.00	811.11	-1.11
.42	.78	.24	1.79	.80	.33	.00	748.00	763.92	-15.92
.15	.63	.28	1.90	.05	.24	.00	794.00	818.50	-24.50
.36	.63	.19	1.84	.06	.23	.00	755.00	766.66	-11.66
.16	.52	.27	3.36	.09	.19	.04	777.00	785.59	-8.59
.18	.79	.21	.52	.56	.19	.00	838.00	824.84	13.16
.30	.80	.29	.54	.55	.21	.00	792.00	801.27	-9.27
.59	.89	.24	.53	.64	.22	.00	745.00	750.41	-5.41
.44	.90	.25	.45	.54	.22	.00	775.00	772.57	2.43
.24	.94	.47	.30	.34	.14	.00	844.00	828.17	15.83
.10	1.63	.21	.00	.00	.41	.00	864.00	845.85	18.15
.63	.87	.17	.02	.04	.00	.02	736.00	741.03	-5.03
.14	.81	.34	1.81	.49	.27	.00	810.00	821.06	-11.06
.16	.60	.27	1.92	.06	.27	.00	800.00	815.36	-15.36
.18	.57	.24	.31	.31	.15	.00	850.00	837.48	12.52
.43	1.02	.26	.31	.48	.13	.00	770.00	774.84	-4.84
.22	.76	.20	.57	.51	.20	.00	832.00	814.51	17.49
.45	.89	.31	.59	.66	.12	.00	773.00	771.24	1.76
.50	.77	.23	.60	.50	.21	.00	755.00	760.83	-5.83
.19	.77	.24	.42	.40	.12	.00	827.00	827.52	-.52
.46	.79	.38	.91	.77	.18	.00	782.00	769.15	12.85
.18	.67	.17	1.07	.00	.00	.00	824.00	816.93	7.07
.19	.75	.18	1.04	.00	.00	.00	823.00	814.26	8.74
.17	1.65	.16	1.07	.00	.00	.00	800.00	797.29	2.71
.21	.75	.18	1.08	.48	.00	.00	811.00	804.19	6.81
.21	.78	.19	1.09	.99	.00	.00	800.00	799.62	.38
.22	.77	.19	1.08	1.91	.00	.00	786.00	790.16	-4.16
.18	.65	.12	1.09	.00	.26	.00	811.00	814.21	-3.21
.21	.70	.15	1.08	.00	.49	.00	823.00	811.54	11.46
.18	.75	.71	1.07	.00	.00	.00	855.00	843.75	11.25
.27	1.12	.00	.00	.00	.00	.00	813.00	802.24	10.76
.37	.77	.15	.04	.98	.21	.00	787.00	787.04	-.04
.22	.79	.24	.03	.08	.50	.02	812.00	833.39	-21.39
.11	.00	1.83	.00	.00	.00	.00	990.00	993.47	-3.47
.40	.00	1.73	.00	.00	.00	.00	860.00	858.46	1.54
.13	.00	.00	.00	2.99	.00	.00	817.00	824.84	-7.84
.41	.00	.00	.00	2.99	.00	.00	787.00	780.34	6.66
.13	.00	.00	.00	.00	.39	.00	875.00	865.31	9.69
.40	.00	.00	.00	.00	.38	.00	795.00	785.89	9.11
.12	3.08	.00	.00	.00	.00	.00	765.00	786.70	-21.70
.37	3.14	.00	.00	.00	.00	.00	725.00	740.59	-15.59
.11	.00	.00	3.28	.00	.00	.00	775.00	767.64	7.36
.37	.00	.00	3.04	.00	.00	.00	733.00	732.96	.04
.11	.00	.00	.00	.00	1.95	.00	902.00	905.11	-3.11
.46	2.94	.00	.00	.00	.00	.00	730.00	728.98	1.02
.22	5.01	.00	.00	.00	.00	.00	730.00	715.64	14.36

Table 4.1(c) Continued

C	Mn	Si	Ni	Cr	Mo	Cu	Expt.T	Calc.T	Residue
.30	2.43	.00	.00	.00	.00	.00	762.00	771.84	-9.84
.00	1.80	.00	.00	2.90	.00	.00	800.00	796.80	3.20
.00	1.70	.00	.00	2.80	.00	.00	800.00	802.10	-2.10
.00	2.00	.00	.00	3.60	.00	.00	800.00	777.20	22.80
.00	1.60	.00	.00	2.50	.00	.00	800.00	811.00	-11.00
.00	3.30	.00	.00	5.50	.00	.00	750.00	697.50	52.50
.00	3.20	.00	.00	4.40	.00	.00	750.00	720.80	29.20
.16	.00	.00	.00	2.40	.00	.00	829.00	824.84	4.16
.17	.00	.00	.00	3.16	.00	.00	820.00	814.38	5.62
.14	.00	.00	.00	3.83	.00	.00	807.00	812.54	-5.54
.15	.00	.00	.00	4.15	.00	.00	804.00	807.02	-3.02
.34	1.06	.20	.75	.23	.02	.00	800.00	781.73	18.27
.51	.23	.17	5.26	.04	.01	.00	710.00	708.71	1.29
.35	.65	.13	1.27	.55	.00	.00	790.00	771.61	18.39
.33	.57	.23	3.26	.85	.09	.00	750.00	750.72	-.72
.29	.21	.06	3.25	1.45	.00	.00	733.00	736.53	-3.53
.35	.44	.14	4.23	1.43	.13	.00	755.00	740.08	14.92
.32	.56	.27	2.37	.74	.51	.00	780.00	778.74	1.26
.33	.51	.00	.82	2.32	.36	.00	792.00	795.75	-3.75
.38	.56	.15	2.42	.74	.46	.00	770.00	762.68	7.32
.40	1.38	.24	.74	.53	.16	.00	785.00	769.45	15.55
.41	.48	.09	1.75	.17	.22	.00	775.00	756.45	18.55
.44	.58	.23	1.40	1.26	.11	.00	775.00	764.08	10.92
.32	.51	.19	3.02	1.37	.48	.00	790.00	790.41	-.41
.38	1.08	.70	.34	.40	.11	.00	804.00	808.78	-4.78
.12	.45	.40	.31	.62	.00	.26	879.00	879.14	-.14
.00	.00	.00	.00	.00	.00	.00	912.00	912.00	.00
.05	.00	.00	.00	.00	.00	.00	883.00	891.79	-8.79
.11	.00	.00	.00	.00	.00	.00	856.00	869.12	-13.12
.16	.00	.00	.00	.00	.00	.00	838.00	851.53	-13.53
.22	.00	.00	.00	.00	.00	.00	821.00	832.00	-11.00
.27	.00	.00	.00	.00	.00	.00	809.00	817.03	-8.03
.33	.00	.00	.00	.00	.00	.00	795.00	800.64	-5.64
.38	.00	.00	.00	.00	.00	.00	786.00	788.29	-2.29
.44	.00	.00	.00	.00	.00	.00	775.00	775.04	-.04
.49	.00	.00	.00	.00	.00	.00	766.00	765.30	.70
.55	.00	.00	.00	.00	.00	.00	757.00	755.20	1.80
.60	.00	.00	.00	.00	.00	.00	749.00	748.08	.92
.66	.00	.00	.00	.00	.00	.00	740.00	741.11	-1.11
.72	.00	.00	.00	.00	.00	.00	734.00	735.86	-1.86
.77	.00	.00	.00	.00	.00	.00	727.00	732.79	-5.79
.00	.49	.00	.00	.00	.00	.00	893.00	894.85	-1.85
.00	.98	.00	.00	.00	.00	.00	875.00	877.70	-2.70
.00	1.48	.00	.00	.00	.00	.00	856.00	860.20	-4.20
.00	1.97	.00	.00	.00	.00	.00	840.00	843.05	-3.05
.00	2.46	.00	.00	.00	.00	.00	825.00	825.90	-.90
.00	.00	.25	.00	.00	.00	.00	927.00	927.82	-.82
.00	.00	.51	.00	.00	.00	.00	946.00	946.09	-.09
.00	.00	.76	.00	.00	.00	.00	967.00	967.16	-.16
.00	.00	1.02	.00	.00	.00	.00	996.00	995.81	.19
.00	.00	1.27	.00	.00	.00	.00	1033.00	1033.93	-.93
.00	.00	1.53	.00	.00	.00	.00	1090.00	1090.13	-.13
.00	.00	.00	.52	.00	.00	.00	885.00	893.28	-8.28

Table 4.1(c) Continued

C	Mn	Si	Ni	Cr	Mo	Cu	Expt.T	Calc.T	Residue
.00	.00	.00	1.05	.00	.00	.00	860.00	874.20	-14.20
.00	.00	.00	1.58	.00	.00	.00	845.00	855.12	-10.12
.00	.00	.00	2.10	.00	.00	.00	832.00	836.40	-4.40
.00	.00	.00	2.63	.00	.00	.00	820.00	817.32	2.68
.00	.00	.00	.00	.37	.00	.00	906.00	905.34	.66
.00	.00	.00	.00	.93	.00	.00	897.00	895.26	1.74
.00	.00	.00	.00	1.31	.00	.00	892.00	888.42	3.58
.00	.00	.00	.00	1.86	.00	.00	883.00	878.52	4.48
.00	.00	.00	.00	2.24	.00	.00	878.00	871.68	6.32
.00	.00	.00	.00	2.80	.00	.00	872.00	861.60	10.40
.00	.00	.00	.00	.00	.43	.00	922.00	916.73	5.27
.00	.00	.00	.00	.00	.86	.00	937.00	930.59	6.41
.00	.00	.00	.00	.00	1.28	.00	956.00	952.50	3.50
.00	.00	.00	.00	.00	1.71	.00	978.00	983.03	-5.03
.00	.00	.00	.00	.00	2.13	.00	1013.00	1020.30	-7.30
.00	.00	.00	.00	.00	2.55	.00	1058.00	1064.48	-6.48
.00	.00	.00	.00	.00	.00	.22	906.00	906.94	-.94
.00	.00	.00	.00	.00	.00	.44	901.00	901.88	-.88
.00	.00	.00	.00	.00	.00	.88	891.00	891.76	-.76
.00	.00	.00	.00	.00	.00	1.32	881.00	881.64	-.64

nucleation and growth rates for ferrite and austenite are different.

Table 4.1a gives the various compositions of the steels and corresponding Ae_3 temperature. For the sake of completion, binary data are also included in the table. The first 19 steels were investigated by Grange [5]. The steels were isothermally transformed at a number of temperature for varying periods of time, up to several hours, such that doubling of holding time did not cause appreciable change in the amount of austenite. The Ae_3 temperature was that at which the last traces of ferrite transformed to austenite.

The next 72 steels have been included from the United States Steels Corporations's diagrams [6] on isothermal transformation of steels. The experimental technique used for the determination of these Ae_3 temperatures was the same as that used by Grange [5]. The Ae_3 temperature and the chemical composition are taken from the tables of Baganis [13].

Aaronson and Domian [7] austenized their next 10 steels at 1300^{o}C for15 minutes and quenched them to get martensite. The steels were then reheated to temperature in the vicinity of suspected Ae_3 temperature and soaked for 15 minutes. As fine unstable martensite constituted the starting structure, 15 minutes at the holding temperature was considered adequate for the establishment of equilibrium. The Ae_3 temperature was taken to lie between the highest temperature at which ferrite remained in the microstructure and the lowest temperature at which it was not present. The Ae_3 temperature was determined with an accuracy of $\pm$3 to $\pm$10^{o}C[5,7] . Hall et. al. [8] homogenized their steels at 1300^{o}C for three days. The samples from these steels were austenized at 1300^{o}C for 15

minutes and then isothermally reacted as long as 24 hours.

The next three steels were taken from Gilmour et. al. [9]. These steels were homogenized at 1200^{o}C for 18 hours and quenched in water to get fully martensite structure. They were reheated to the holding temperature, isothermally transformed for three days and quenched in water. Austenite in equilibrium with ferrite was considered to have the holding temperature as its Ae_3 temperature. The composition of the austenite was determined by microprobe analysis. The next six steels are taken from Kirchner and Uhrenius [10] who allowed the isothermal transformation to take place in Fe-Cr-Mn alloys for times ranging from one weeks to seven months. From their results, the austenite in equilibrium with ferrite at a particular isothermal transformation temperature was considered to have the isothermal temperature as its Ae_3 temperature. In this case also, the composition was determined by microprobe analysis. Carbon content in these steels was less than 0.004%. Carbon concentration in these alloys is ,therefore, taken to be zero. Swinden and Woodhead [14] austenized their four (next four in the table) Fe-C-Cr steels at 1000^{o}C and then allowed isothermal transformation to take place for several hours. Table 4.1 also lists next fifteen steels whose Ae_3 temperatures were experimentally determined by isothermal transformation[6].

Ae_3 temperatures of binary Fe-C, Fe-Mn, Fe-Si, Fe-Ni, Fe-Mo, and Fe-Cu alloys steels used in the last chapter have been reproduced in Table 4.1a.

In all , 177 alloys of known compositions are selected for which reliable values of Ae_3 temperatures are available. The ranges of weight percentages of the alloying elements in these steels and

the range of their Ae_3 temperatures in ^{o}C are given below;

	Alloying Elements (Wt%)							
	X_C	X_{Mn}	X_{Si}	X_{Ni}	X_{Cr}	X_{Mo}	X_{Cu}	Ae_3 Temp(^{o}C)
Minimum Value	0	0	0	0	0	0	0	712
Maximum Value	0.758	5.00	1.83	5.26	5.50	2.549	1.49	1090

4.4 Evaluation of the Coefficients of the Model:

A polynomial series after fourth order is truncated for the model. This contains 7 terms of the first order, 28 terms of the second order, 84 terms of the third order and 210 terms of the fourth order besides the zeroth order constant and all these make 329 terms excluding the constant term. The task is to determine the coefficients in the model.

We know that the Ae_3 temperature of pure iron is $912^{o}C$. Hence the constant term was forced to be 912. The values of the remaining desirable coefficients are to be determined by using the Ae_3 temperatures of the 177 steels listed in Table 4.1a.

4.4.1 Significance Levels:

We have already discussed the use of regression to compute the coefficients of a model in chapter II. Here, the number of coefficients in the model are very large at 329. As suggested there, the stepwise regression analysis is used in such case as stepwise regression screens out the less significant variables in a model. The details of the principles of stepwise multiple regression are available in standard texts[15,16,17,18] and its elementary ideas were discussed in chapter II. Here we mention just significance level which is important for our purpose. The significance level is a statistical parameter which gives the probability of the variable

not being a predictor variable. The minimum significance level (α_{entry}) , beyond which a variable is considered unsuitable for inclusion in the regression equation , need to be specified. The maximum significance level (α_{stay}) up to which a variable can be retained in the regression equation also has to be fixed. In our case, we have set both α_{entry} and α_{stay} equal as Draper and Smith [14] has suggested that it is usually the best to set the both as equal. The process of adding and removing the variables is continued until no more variables will be admitted to the equation and no more are rejected [15]. Thus, for a particular set of significance levels specified for the entering and leaving variables, a best set of coefficients can be calculated.

A standard program RSTEP available with IMSL library was used to evaluate the coefficients of this model. The calling program has been listed in Appendix I. The results obtained with various sets of α_{entry} and α_{stay} are listed in Table 4.2.

The data in Table 4.2 show that there is hardly any difference between the results obtained by changing α from 0.01 to 0.07. Figures 4.1(a,b) to Figures 4.3(a,b), which show plots of expt. vs calc. Ae_3 temperature, cumulative frequency curve and frequency density curve, also confirm equivalents of results obtained with two sets of values of α. However, the coefficients are 18 when α is 0.01 while those for the rest of the values of α are 23.

4.4.2 Coefficients of the Model:

The coefficients obtained with α = 0.01 and α = 0.03 are listed in Table 4.3. The table also lists the variables. It is clear from the table that the variables which appear with α = 0.01 also appear when α = 0.05. However, for α = 0.05 , five new variables make their

Table 4.7

Statistical Parameters for Different Significance Level

Significance Level		Total no. of Coefficients	SF	Residue		Multiple Correlation Coefficients
α_{entry}	α_{stay}			Min.	Max.	
0.01	0.01	18	9.5	25.70	34.79	99.04834%
0.03	0.03	23	8.9	26.48	35.59	99.11240%
0.05	0.05	23	8.9	26.48	35.59	99.14240%
0.07	0.07	23	8.9	26.48	35.59	99.14249%

Table 4.3

Coefficients of the Model Equations with no Binary Coefficients Fixed for α = 0.01 and α = 0.03

Variable	Coefficients For α_{entry} α_{stay} = 0.01	Coefficients For α_{entry} α_{stay} = 0.03
X_C	4.175×10^{4}	4.230×10^{4}
X_{Mn}	3.628×10^{3}	3.683×10^{3}
X_{Si}	9.360×10^{3}	9.308×10^{3}
X_{Ni}	3.353×10^{3}	3.568×10^{3}
X_{Cr}	1.674×10^{3}	1.678×10^{3}
X_{Mo}	1.920×10^{3}	2.217×10^{3}
X_{Cu}	1.480×10^{3}	2.361×10^{3}
X_C^2	2.437×10^{6}	2.476×10^{6}
$X_C X_{Mn}$	8.220×10^{6}	8.356×10^{5}
$X_C X_{Si}$	1.260×10^{6}	1.243×10^{6}
$X_C X_{Ni}$	3.584×10^{5}	5.244×10^{5}
$X_C X_{Cr}$	3.978×10^{5}	4.155×10^{5}
$X_C^2 X_{Mn}$	6.779×10^{7}	6.409×10^{7}
$X_{Mn}^2 X_{Ni}$	-	8.541×10^{6}
$X_{Si}^2 X_{Cu}$	-	4.364×10^{8}
X_{Mo}^3	6.068×10^{6}	5.503×10^{6}
$X_C X_{Mn} X_{Ni}^2$	-	1.336×10^{9}
$X_C X_{Mn} X_{Ni} X_{Cr}$	3.379×10^{9}	1.005×10^{9}
$X_C X_{Mo}^3$	6.399×10^{9}	6.466×10^{9}
$X_{Mn} X_{Si} X_{Ni} X_{Mo}$	-	1.141×10^{10}
$X_{Mn} X_{Ni}^3$	4.742×10^{7}	8.889×10^{7}
$X_{Mn} X_{Cr}^3$	9.450×10^{6}	9.919×10^{6}
$X_{Ni} X_{Cr} X_{Mo}$	-	8.971×10^{8}

appearance. This is expected as the α is increased. However , when α is increased from 0.03 to 0.07, the variables which appear are identical.

The variables in this table are in the form of weight fraction. However, it is practically more useful to express it in weight percentage. Therefore, the coefficients in table 4.3 are expressed below in equation containing weight percentages of elements,where the weight percentage of an element i is represented by W_i.

Equation for α = 0.01

$$T_e = 912 - 417.5\,W_C - 36.28\,W_{Mn} + 93.6\,W_{Si} - 33.53\,W_{Ni} - 16.74\,W_{Cr} + 19.2\,W_{Mo} - 14.8\,W_{Cu} + 243.7\,W_C^2 + 82.2\,W_C\,W_{Mn} - 126\,W_C\,W_{Si} + 35.84\,W_C\,W_{Ni} + 39.78\,W_C\,W_{Cr} - 67.79\,W_C^2\,W_{Mn} + 6.068\,W_{Mo}^3 + 33.79\,W_C W_{Mn} W_{Ni} W_{Cr} - 63.99\,W_C\,W_{Mo}^3 + 0.4742\,W_{Mn} W_{Ni}^3 + 0.0945\,W_{Mn} W_{Cr}^3$$

Equation for α = 0.03

$$T_e = 912 - 423\,W_C - 36.83\,W_{Mn} + 93.08\,W_{Si} - 35.68\,W_{Ni} - 16.78\,W_{Cr} + 22.17\,W_{Mo} - 23.618\,W_{Cu} + 247.6\,W_C^2 + 83.56\,W_C\,W_{Mn} - 124.3\,W_C\,W_{Si} + 52.44\,W_C\,W_{Ni} + 41.55\,W_C\,W_{Cr} - 64.09\,W_C^2\,W_{Mn} + 8.541\,W_{Mn}^2 W_{Ni} + 436.4\,W_{Si}^2 W_{Cu} + 5.503\,W_{Mo}^3 - 13.36\,W_C W_{Mn} W_{Ni}^2 + 10.05\,W_C W_{Mn} W_{Ni} W_{Cr} - 64.66\,W_C W_{Mo}^3 - 114.1\,W_{Mn} W_{Si} W_{Ni} W_{Mo} + 0.8889\,W_{Mn} W_{Ni}^3 + 0.09919\,W_{Mn} W_{Cr}^3 + 8.971\,W_{Ni}^2 W_{Cr} W_{Mo}$$

We note that $W_i = 100\,X_i$, Where X_i is the weight fraction

4.5 Comparison with Existing Models:

Table 4.4 contains values of the mean of residue, number of steels used in a model, standard error of estimate, minimum and maximum values of the residue and the coefficients of multiple correlation for all the models [5,12,13]. 177 alloys were used for the present model and 173 for Grange's [5] model. The parameters for

the Baganis [13] model were determined for 171 steels. For Andrews [12] model, 13steels could not be included as his table does not have provision for steels with [C + Ni/10] greater than 0.7% . The number of alloys considered for each model is listed in the table 4.4.

We can see from the table 4.4 that coefficient of correlation is the highest for the present case. Also, the range of residue is minimum and standard error of estimate is the least. Mean of residue is also small for our case but it is minimum for Andrews [12] model but then standard error of estimate is larger than ours.

The frequency density distribution of the residue for all the models, in fig.4.3(a,b) and 4.6, suggest that the distributions for the models available in the literature are relatively asymmetric and the spreads are large. The cumulative frequency curves for the residues from all the models are shown in fig.4.2(a,b) and 4.5.

The plot-backs for the models are shown in figures 4.1(a,b,c) and figures 4.4(a,b,c). A comparison of these plots with that of the present model shows that the dispersion of the points about the 45^{o} line is minimum for the present model. The present models thus appear to be much more satisfactory than all the existing models.

4.6 Comparison of the Results of Stepwise Regression of Multicomponent Data with Those of Binary Data:

When the expression for Ae_3 temperature derived after stepwise regression is reduced to those applicable to binary data we obtain the following expressions:

Equation for $\alpha = 0.01$

$$T_e = 912 - 417.5\ W_C + 243.7\ W_C^2$$

$$T_e = 912 - 36.28\ W_{Mn}$$

Table 4.4

Statistical Analysis of the Results from Different Models for Ae_3 Temperature

Description	Model with α = 0.01	Model with α = 0.03	Baganis' model [13]	Andrews' model [12]	Grange's model [5]
No. of steels considered	177	177	171	160	173
Mean of residue	-0.53	-1.42	9.60	0.2	17.2
SE	9.5	8.9	13.8	19.2	33.3
Residue (Min.)	-25.70	-26.48	-16.8	-76.8	-52.4
Residue (Max.)	34.79	35.59	50.1	85.1	203.6
Coefficient of correlation	.9904325	.9914249	.977	.961	.909

$T_e = 912 + 93.6\ W_{Si}$

$T_e = 912 - 33.53\ W_{Ni}$

$T_e = 912 - 16.74\ W_{Cr}$

$T_e = 912 + 19.2\ W_{Mo} + 6.068\ W_{Mo}^3$

$T_e = 912 - 14.8\ W_{Cu}$

Equation for $\alpha = 0.03$

$T_e = 912 - 423\ W_C + 247.6\ W_C^2$

$T_e = 912 - 36.83\ W_{Mn}$

$T_e = 912 + 93.08\ W_{Si}$

$T_e = 912 - 35.68\ W_{Ni}$

$T_e = 912 - 16.78\ W_{Cr}$

$T_e = 912 + 22.17\ W_{Mo} + 5.503\ W_{Mo}^3$

$T_e = 912 - 23.618\ W_{Cu}$

Comparison of these equations with those [Table 3.2.] obtained by using binary data shows that the stepwise regression yields equations which are much simpler and mostly contain first order except, C and Mo. However, in all set of equations the austenite stabilizers depress the Ae_3 temperature while the ferrite stabilizers increase it. Cr is an exception which first depresses and then increases the Ae_3 temperature. From the Fe-Cr phase diagram[figure 2.5], this behaviour is expected.

Comparison of the residue obtained from the binary equations (table 3.1) with those obtained from the stepwise regression (table4.1) shows that the error are much more with the stepwise regression. This is expected because the analysis gives equal weightage to all the data. Although the binary data are expected to be much more accurate than the multicomponent data.

Table 4.5 lists the ranges of residues in all the binary data

Table 4.5

Ranges of Residue corressponding to Binary Data for Model Equations with $\alpha = 0.01$ and $\alpha = 0.03$

Systems	Model with No coefficients Fixed $\alpha = 0.01$		Model with No Coefficients Fixed $\alpha = 0.03$	
	Residue		Residue	
	Min.	Max.	Min.	Max.
Fe-C	-13.44	0.91	-12.66	2.75
Fe-Mn	-2.31	2.25	-1.49	3.60
Fe-Si	-16.14	34.79	-15.74	35.59
Fe-Ni	-16.79	-3.82	-14.54	1.84
Fe-Cr	0.19	6.87	0.21	6.98
Fe-Mo	-3.58	6.70	-1.78	4.08
Fe-Cu	-11.46	-2.74	-0.81	0.17

due to multiple regression. It is clear that the equations obtained by stepwise regression using $\alpha = 0.03$ gives reasonable fit with reasonable scatter in the Fe-Cu, Fe-Mo, Fe-Cr and Fe-Mn systems. In the Fe-C and Fe-Ni systems the scatter is also not too high except for a couple of points which are above 10. The Fe-Si system , however, shows considerable scatter.It is possible that this scatter is inherent to the Fe-Si system itself. However, in order to reduce the scatter in the predicted Ae_3 temperatures of binary Fe-Si alloys, multiple stepwise regression was tried after keeping the coefficients obtained from binary Fe-Si data fixed in stepwise multiple regression of the data.

4.6.1 Stepwise Multiple Regression Keeping the Coefficients Obtained from the Binary Fe-Si Alloys Fixed:

From the section on binary alloys we know that the Ae_3 temperature of binary Fe-Si can be accurately described by the following equation:

$$T_e = 912 + 61\ W_{Si} + 8.37\ W_{Si}^2 + 11.9\ W_{Si}^4 \quad ; SE = 0.39^{\circ}C$$

In the stepwise linear regression, therefore, the following coefficients were kept fixed:

(1) $A = 912$

(2) $A = 6100$

(3) $A_{SiSi} = 8.37 \times 10^4$

(4) $A_{SiSiSi} = 0$

(5) $A_{SiSiSiSi} = 11.9 \times 10^8$

Keeping the above coefficients fixed and using the 177 data points, multiple stepwise regression was carried out as before. Several significance levels, 0.005, 0.007, 0.009, 0.01 and 0.03, were tried. It was found that when the significance level was 0.005, 0.007 and

0.009, the number of coefficients and other statistical parameters such as estimated standard deviation of model error were found to be identical. When α was increased appreciably i.e. to 26. Therefore, α = 0.005 was chosen.

Using the significance level of 0.005, stepwise multiple regression analysis gave the coefficients listed in Table 4.6 . Comparison of these coefficients with those obtained without keeping the coefficients obtained from the binary Fe-Si alloys fixed shows that the binary coefficients have hardly changed except that there is no linear term in Mo and a number of cross terms have been replaced by new ones that contain primarily silicon.

The calculated Ae_3 temperatures using this model and the residue are listed in Table 4.1c. It shows that the residues have not been appreciably changed except for one steel containing Mn = 3.3%, Cr = 5.5% for which residue is 52.5. For the same steel, the residue after multiple regression without keeping any binary coefficients fixed is -2.63 (Table 4.1a). However, the frequency density distribution of residues show that the negative residue have been reduced considerably. However, on positive side, there are few high values.

The statistical parameters and the number of coefficients are listed in Table 4.7, which also lists the results of stepwise regression where no binary coefficients were fixed. The comparison shows that the models are almost equally good, except that frequency density distribution becomes a little more asymmetric when coefficients in Table 4.6 is used.

Stepwise regression keeping the binary coefficients obtained from the binary Fe-C, Fe-Si and Fe-Ni alloys were also tried with α

Table 4.6

Coefficients of Model Equation when Binary Si Coefficients are Fixed for $\alpha = 0.005$

Terms	W_C	W_{Mn}	W_{Si}	W_{Ni}	W_{Cr}	W_{Cu}
Coefficients	-416	-35	61	-36	-18	-23
Terms	W_C^2	$W_C W_{Mn}$	$W_C W_{Ni}$	$W_C W_{Cr}$	W_{Si}^2	$W_{Si} W_{Ni}$
Coefficients	238	91	46	43	8.37	43
Terms	W_{Mo}^2	$W_C^2 W_{Si}$	W_{Mo}^3	$W_C^2 W_{Mn}$	$W_C^2 W_{Si}^2$	$W_C W_{Si}^3$
Coefficients	26	522	-1	-34	1139	-272
Terms	$W_C W_{Si}^2 W_{Ni}$	$W_C W_{Mo}^3$	$W_{Mn} W_{Cr} W_{Cu}^2$	W_{Si}^4	$W_{Ni} W_{Cr}^2 W_{Mo}$	
Coefficients	-300	-68	1105	11.9	14	

Table 4.7

Comparision of Statistical Parameters of Different Models

Description	Model with fixed Binary Si Coefficients α = 0.005	Model with fixed Binary C,Si,Ni Coe ficients α = 0.005	Binary Coefficients not fixed α = 0.03
No. of Coefficients	23	31	23
Mean of residue	-0.04	3.02	-1.42
SE	9.57	19.10	8.9
Residue (Min.)	-24.5	-22.58	-26.48
Residue (Max.)	52.50	152.05	35.59
Coefficient of correlation	99.0322%	95.9856%	99.14349%

= 0.005. Number of Coefficients and other statistical parameters obtained from this model are also listed in the Table 4.7. However, the results are not satisfactory and hence ignored.

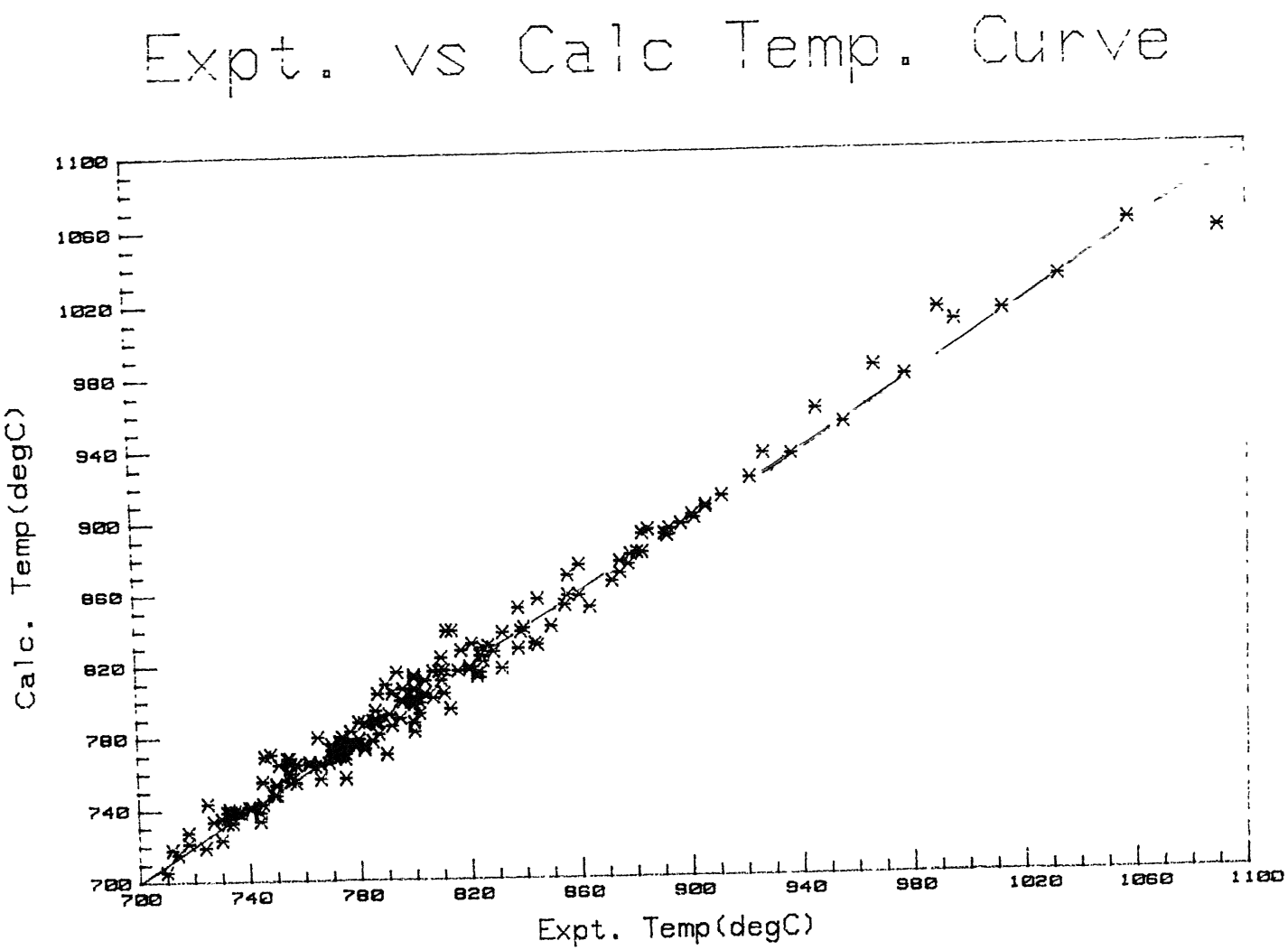


Fig. 4.1(a) Scattergram for the Model with α = 0.03 and No Binary Coefficients Fixed

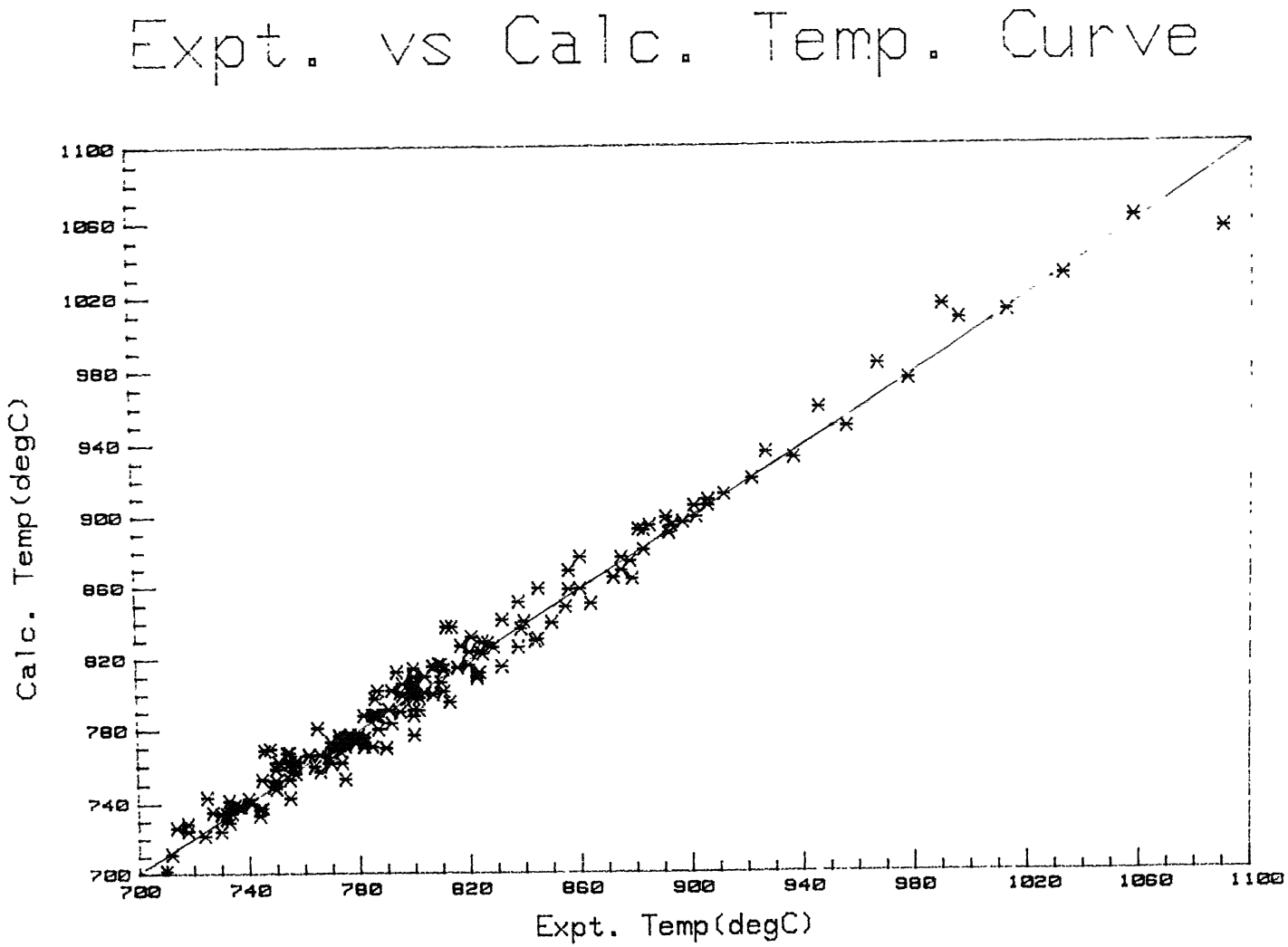


Fig. 4.1(b) Scattergram for the Model with α = 0.01 and No Binary Coefficients Fixed

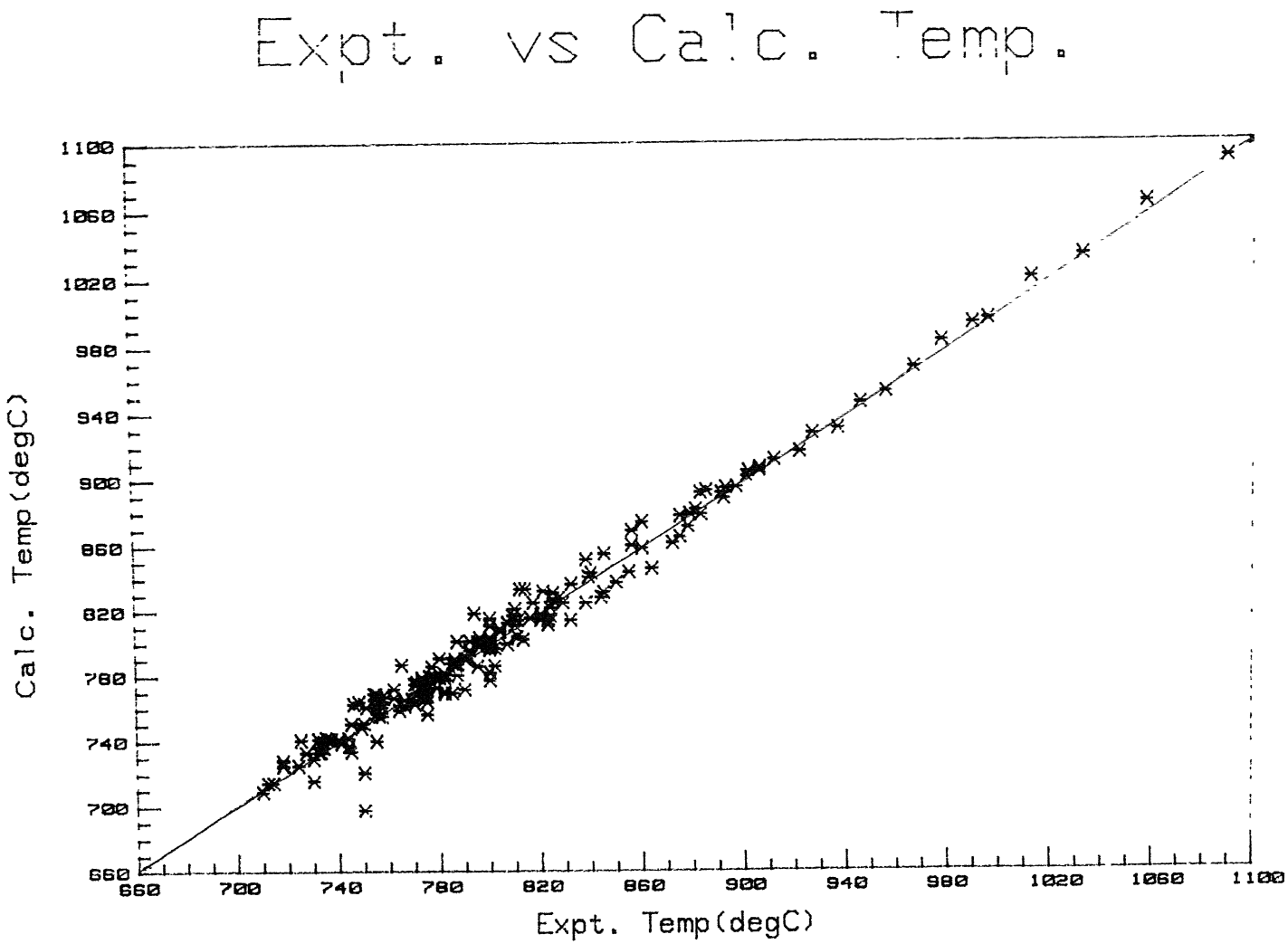


Fig. 4.1(c) Scattergram for the Model with α = 0.005 and Binary Si Coefficients Fixed

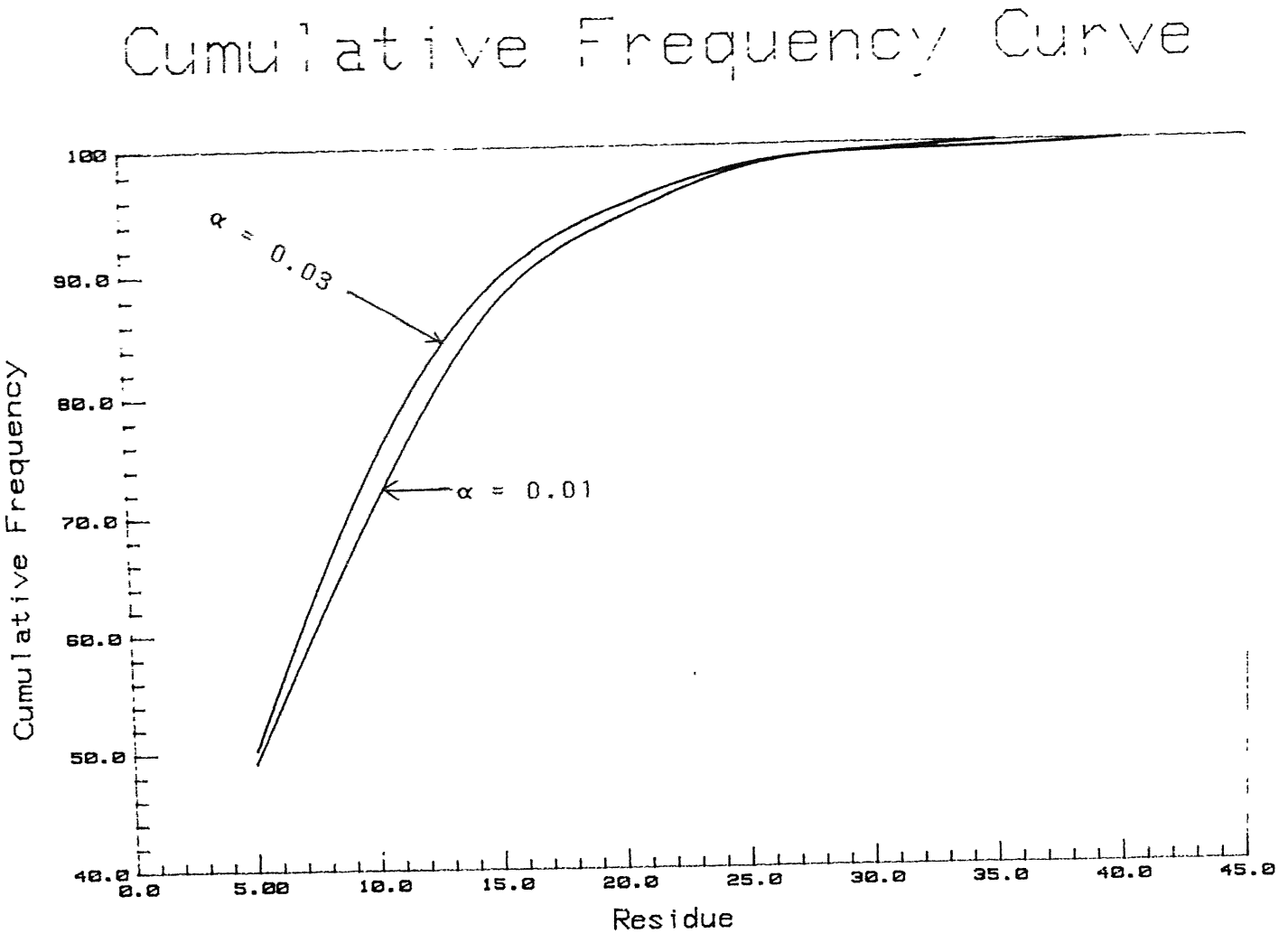


Fig. 4.2(a) Cumulative Frequency Distribution for Residue

with $\alpha = 0.01$ and $\alpha = 0.03$ and no Binary Fixed

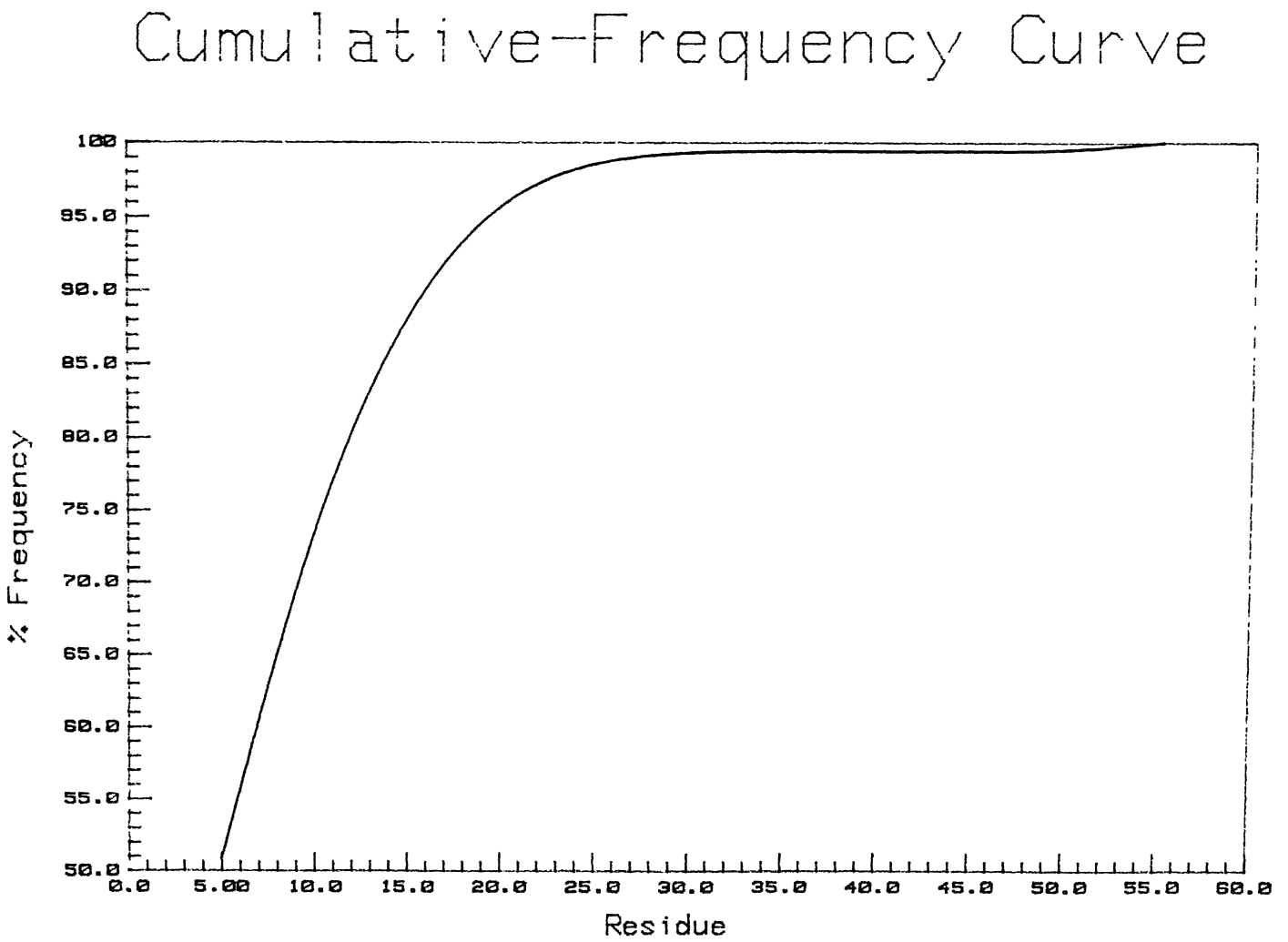


Fig. 4.2(b) Cumulative Frequency Distribution for Residue

with Fixed Binary Coefficients of Si with $\alpha = 0.005$

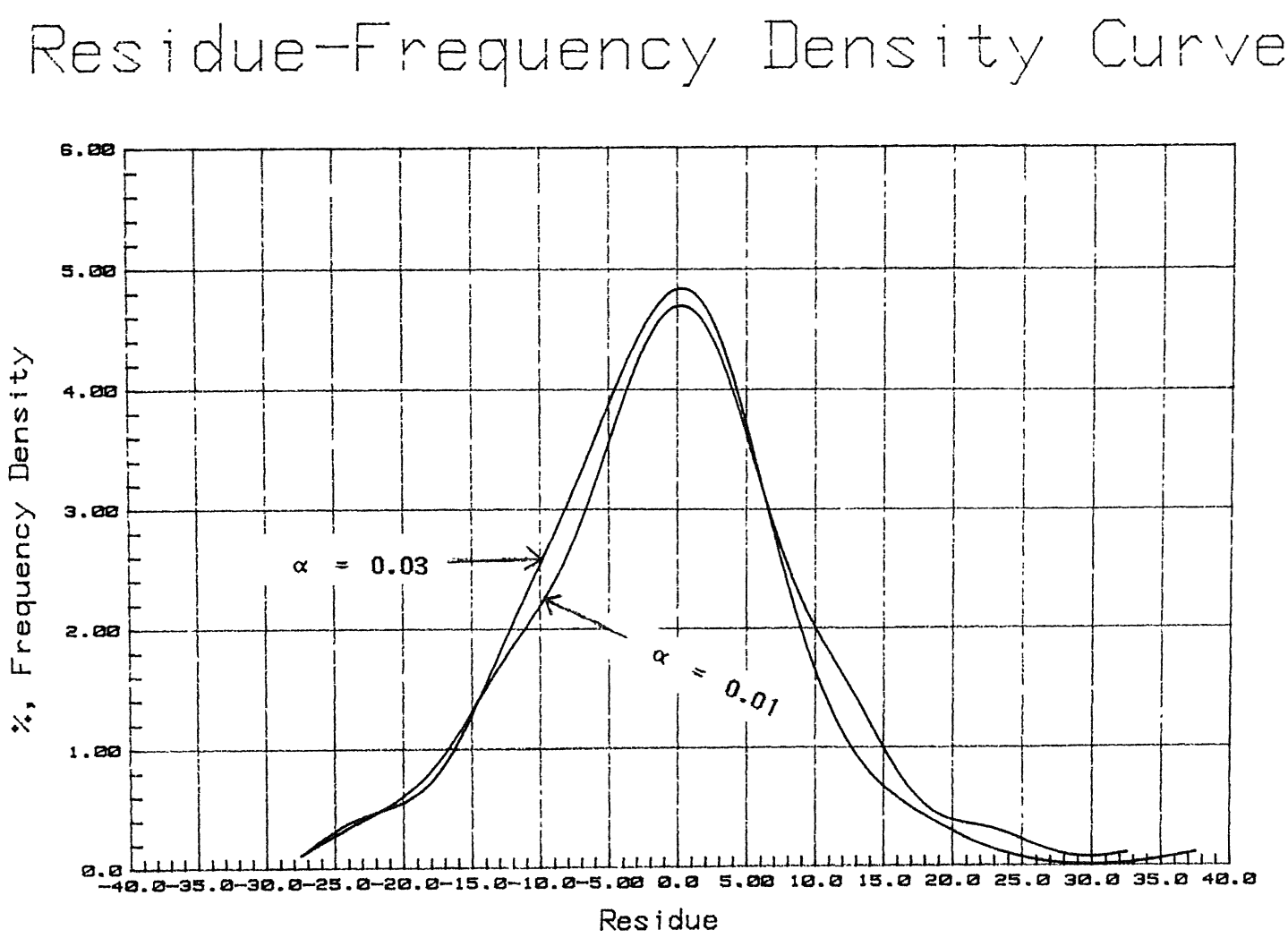


Fig. 4.3(a) Frequency Density Distribution Curve for Residue with $\alpha = 0.01$ and $\alpha = 0.03$ and no Binary Fixed

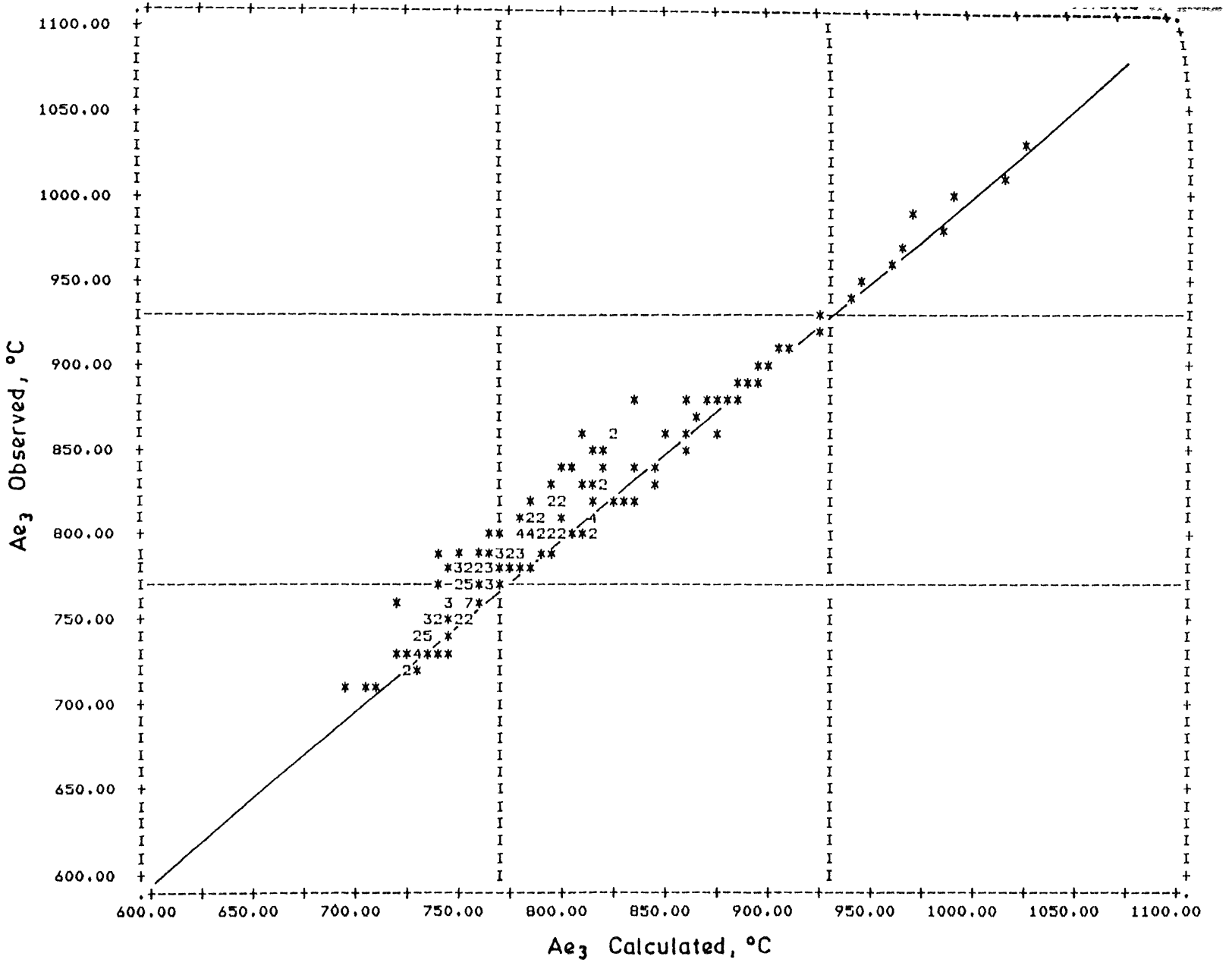


Fig. 4.4(a) Scattergram for the Baganis' Model

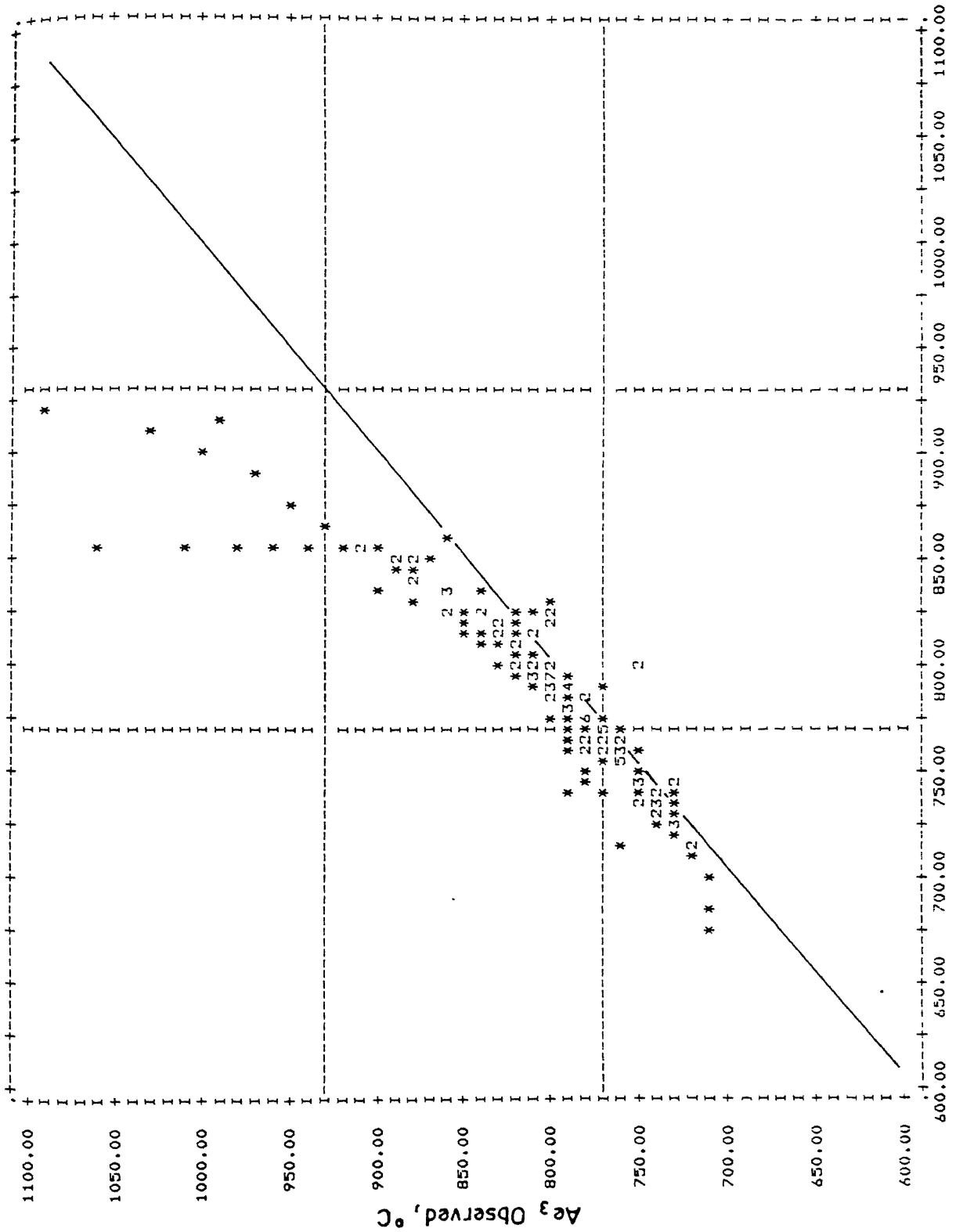


Fig. 4.4(b) Scattergram for the Grange's Model

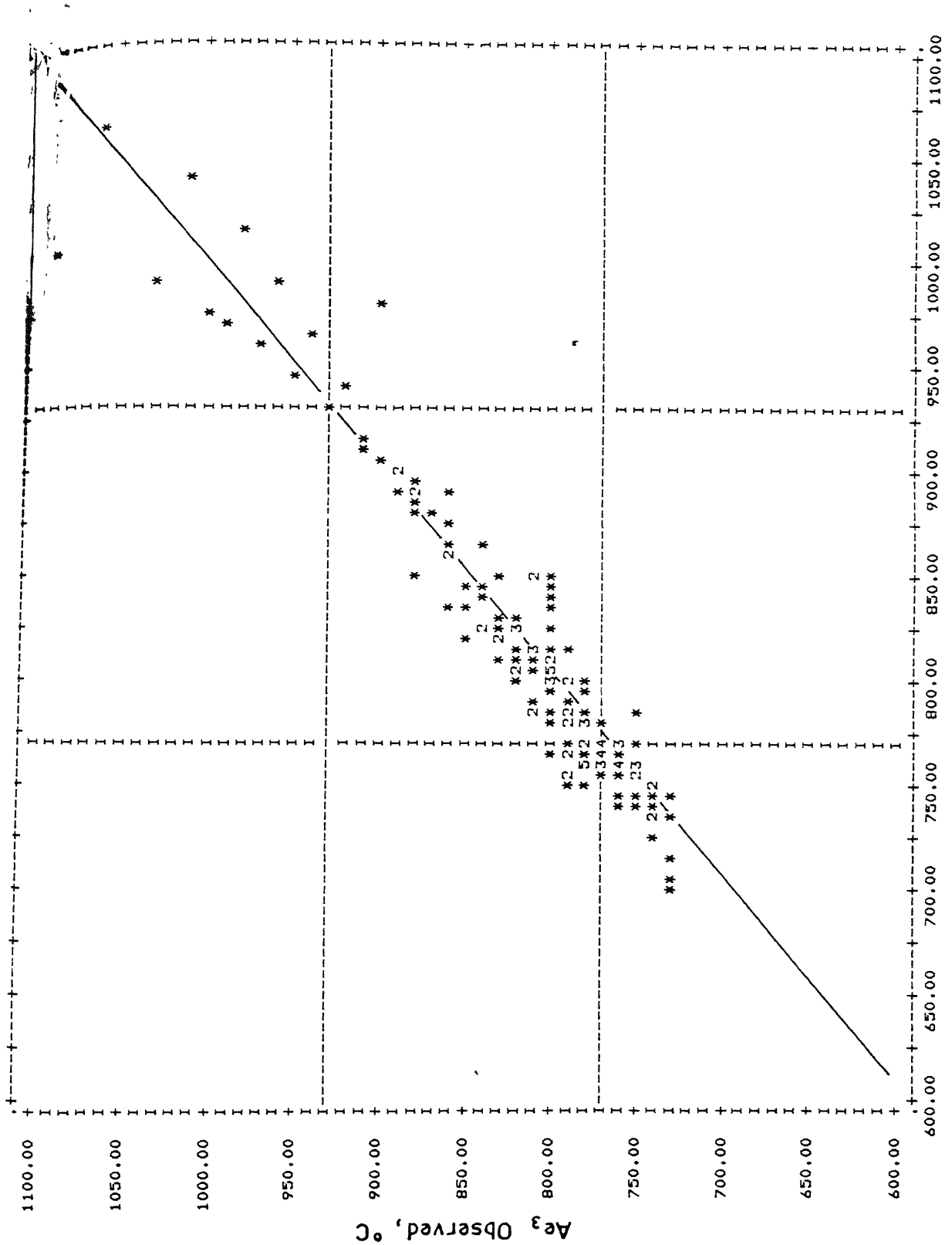


Fig. 4.4(c) Scattergram for the Andrew's Model

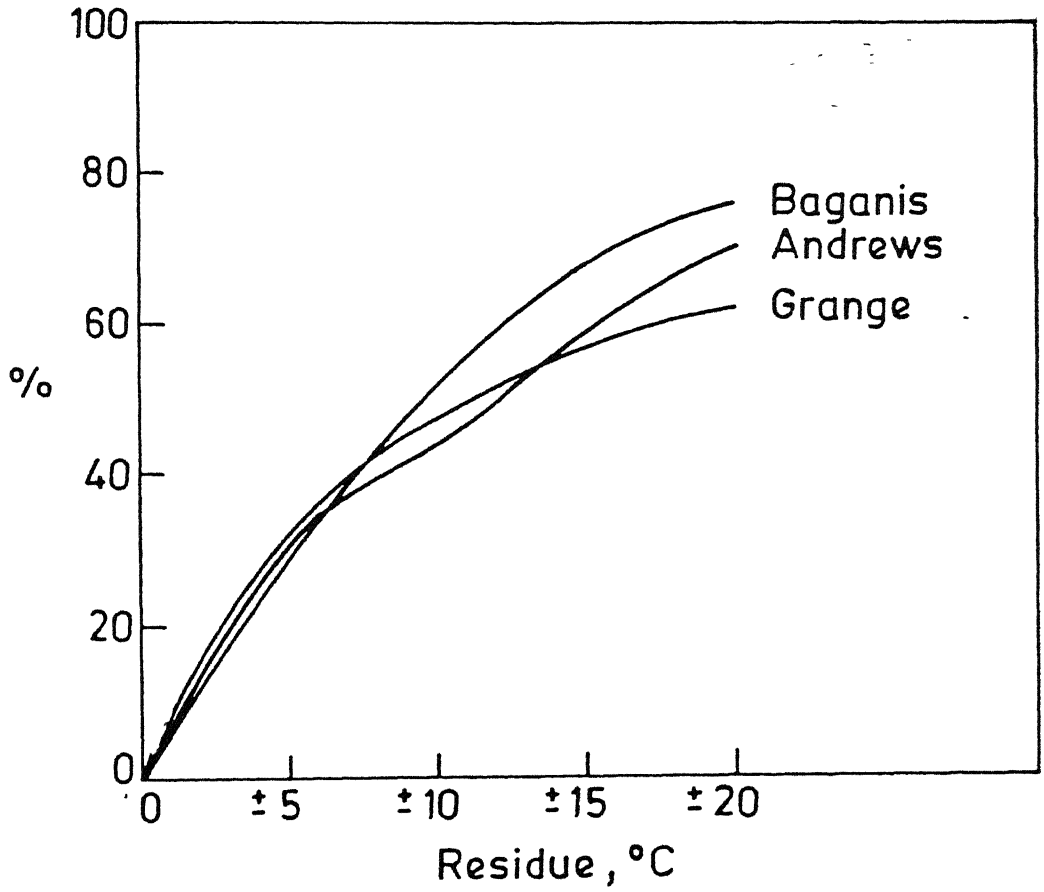


Fig. 4.5 Cumulative Frequency Distribution for Residue from different Models

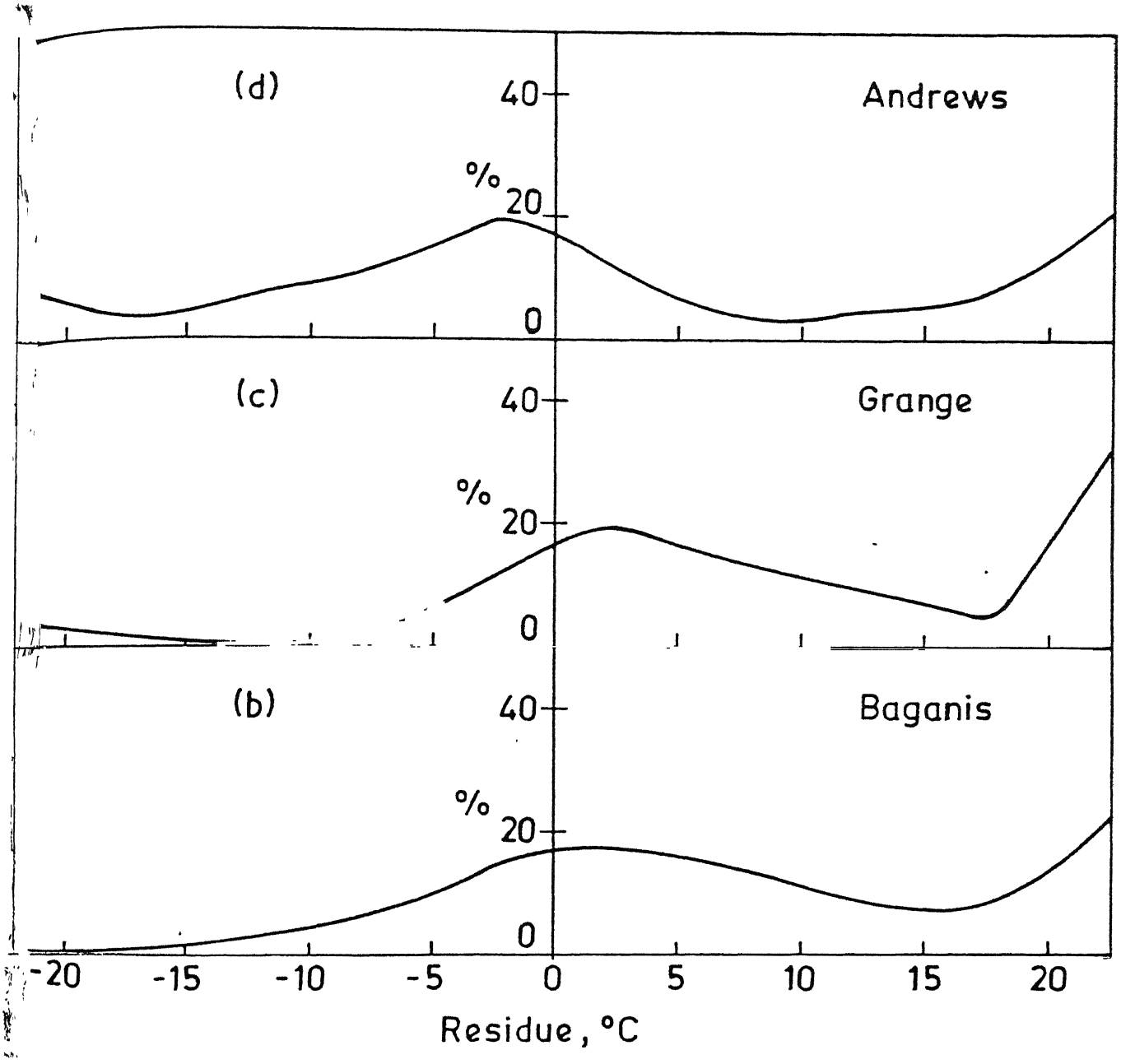


Fig. 4.6 Frequency Distribution for Residue from different Models

CHAPTER V

SUMMARY AND CONCLUSION

1. Equations were developed to correlate Ae_3 temperatures with composition of steels.

2. 177 accurately determined data points were selected from the literature. The Ae_3 temperatures and the corresponding steels compositions were recorded.

3. The data available on seven binary systems , Fe-C, Fe-Mn, Fe-Si, Fe-Ni, Fe-Cr, Fe-Mo and Fe-Cu, were curve fitted and the following relations were obtained:

Fe-C: $T_e = 912 - 526W_C + 528W_C^2 + 272W_C^4$; $\sigma = \pm 2.48^oC$

Fe-Mn: $T_e = 912 - 38.7W_{Mn} + 0.41W_{Mn}^2 + 0.155W_{Mn}^4$; $\sigma = \pm 0.28^oC$

Fe-Si: $T_e = 912 + 61W_{Si} + 8.37W_{Si}^2 + 11.9W_{Si}^4$; $\sigma = \pm 0.39^oC$

Fe-Ni: $T_e = 912 - 61.6W_{Ni} + 12.8W_{Ni}^2 + 0.397W_{Ni}^4$; $\sigma = \pm 0.78^oC$

Fe-Cr: $T_e = 912 - 15.6W_{Cr} - 0.231W_{Cr}^2 + 0.0901W_{Cr}^4$; $\sigma = \pm 0.28^oC$

Fe-Mo: $T_e = 912 + 22.8W_{Mo} + 6.71W_{Mo}^2 + 1.05W_{Mo}^4$; $\sigma = \pm 0.80^oC$

Fe-Cu: $T_e = 912 - 27.8W_{Cu} + 7.25W_{Cu}^2 - 2.99W_{Cu}^3$; $\sigma = \pm 0.10^oC$

4. From the discussion in chapter iv,it is concluded that the following equation

$$T_e = 912 - 423\ W_C - 36.83\ W_{Mn} + 93.08\ W_{Si} - 35.68\ W_{Ni} - 16.78\ W_{Cr} + 22.17\ W_{Mo} - 23.618\ W_{Cu} + 247.6\ W_C^2 + 83.56\ W_C\ W_{Mn} - 124.3\ W_C\ W_{Si} + 52.44\ W_C\ W_{Ni} + 41.55\ W_C\ W_{Cr} - 64.09\ W_C^2\ W_{Mn} + 8.541\ W_{Mn}^2 W_{Ni} + 436.4\ W_{Si}^2 W_{Cu} + 5.503\ W_{Mo}^3 - 13.36\ W_C W_{Mn} W_{Ni}^2 + 10.05\ W_C W_{Mn} W_{Ni} W_{Cr} - 64.66\ W_C W_{Mo}^3 - 114.1\ W_{Mn} W_{Si} W_{Ni} W_{Mo} + 0.8889\ W_{Mn} W_{Ni}^3 + 0.09919\ W_{Mn} W_{Cr}^3 + 8.971\ W_{Ni}^2 W_{Cr} W_{Mo} \quad ; \quad \sigma = \pm 8.9^oC$$

which is obtained without keeping any binary coefficients fixed and

the following equation,

$$T_e = 912 - 416\,W_C - 35\,W_{Mn} + 61\,W_{Si} - 36\,W_{Ni} - 18\,W_{Cr} - 23\,W_{Cu}$$
$$+ 238\,W_C^2 + 91\,W_C W_{Mn} + 46\,W_C W_{Ni} + 43\,W_C W_{Cr} + 8.37\,W_{Si}^2$$
$$+ 43\,W_{Si} W_{Ni} + 26\,W_{Mo}^2 - 522\,W_C^2 W_{Si} - W_{Mo}^3 - 34\,W_C^2 W_{Mn}^2$$
$$+ 1139\,W_C^2 W_{Si}^2 - 272\,W_C W_{Si}^3 - 300\,W_C W_{Si}^2 W_{Ni} - 68\,W_C W_{Mo}^3$$
$$+ 1105\,W_{Mn} W_{Cr} W_{Cu}^2 + 11.9\,W_{Si}^4 + 14\,W_{Ni} W_{Cr}^2 W_{Mo} \; ; \; \sigma = \pm 9.57^{\circ}C$$

which is obtained by keeping the coefficients obtained by binary Fe-Si alloys fixed , are equally satisfactory in predicting the Ae_3 temperature.

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APPENDIX I

```
*         stepwise  regression analysis
*
        EXTERNAL  RSTEP,MXTXF
*
*
           REAL     DATAM,B
        DIMENSION  DATAM(177,330),B(330,330),LEVEL(330)
        DIMENSION  SCALE(330),HIST(330),AOV(13),COEF(329,5)
        DIMENSION  COVS(330,330)
        DIMENSION  L1(330),L2(330),L3(330),L4(330),L5(330)
*
           NV =329
        NDATA = 177
        READ(*,*) SL1,SL2
**********************
*          reading data in the matrix DATAM
**********************
        READ(*,*) ( (DATAM(I,J),J =1,8),I =1,NDATA)
        DO  11 I=1,NDATA
            DATAM(I,8) = DATAM(I,8) - 912.
 11     CONTINUE
*
*
*
**********************
*          creating additional data in DATAM
**********************
*
*
* ........................
* ....... 2ND degree polynomial data generation 00
* ........................
          NC = 9
          DO 10 I = 1,7
            DO 20 J = I,7
             DO 30 K = 1,NDATA
                DATAM(K,NC) = DATAM(K,I)* DATAM(K,J)
 30          CONTINUE
               L1(NC-8) = NC
               L2(NC-8) = I
               L3(NC-8) = J
               NC = NC +1
 20          CONTINUE
 10       CONTINUE
               NC2 = NC
*
* ........................
* .......>3RD degree polynomial data generation 000
* ........................
*
        DO 100 I1 = 1,7
         DO 200 I2 = I1,7
          DO 300 I3 = I2,7
```

```
            DO 400 J = 1,NDATA
              DATAM(J,NC)= DATAM(J,I1)*DATAM(J,I2)*DATAM(J,I3)
 400        CONTINUE
               L1(NC-8) = NC
               L2(NC-8) = I1
               L3(NC-8) = I2
               L4(NC-8) = I3
               NC =NC+1
 300       CONTINUE
 200      CONTINUE
 100     CONTINUE
*
* .......................
* ...... 4TH degree polynomial data genaration 001
* .......................
*
        DO 101 I1 = 1,7
         DO 102 I2 = I1,7
          DO 103 I3 = I2,7
           DO 104 I4 = I3,7
            DO 105 J = 1,NDATA
             DATAM(J,NC) = DATAM(J,I1) * DATAM(J,I2) *
     1                     DATAM(J,I3) * DATAM(J,I4)
 105        CONTINUE
                L1(NC-8) = NC
                L2(NC-8) = I1
                L3(NC-8) = I2
                L4(NC-8) = I3
                L5(NC-8) = I4
                NC = NC + 1
 104       CONTINUE
 103      CONTINUE
 102     CONTINUE
 101    CONTINUE
*
*
*
**********************
*       calling routine MXTXF
**********************
*
        CALL  MXTXF(NDATA,NV,DATAM,NDATA,NV,B,NV)
*
**********************
*       processing data for RSTEP
**********************
        INVOKE = 0
        DATA  LEVEL /7*1,-1,322*1/
        NFORCE = 0
        NSTEP = -1
        ISTEP = 1
        NOBS = NDATA + 1
        PIN  = SL1
        POUT = SL2
        TOL = 100. * AMACH(4)
        IPRINT = 1
*
```

```
*********************
*       calling routine RSTEP
*********************
*
        CALL RSTEP(INVOKE,NV,B,NV,LEVEL,NFORCE,NSTEP,
     1       ISTEP,NOBS,PIN,POUT,TOL,IPRINT,SCALE,HIST,
     1       IEND,AOV,COEF,NV-1,COVS,NV)
*
*
           DO 110 I =1,13
           WRITE(*,*) AOV(I)
110     CONTINUE
*
*
         WRITE(*,*)'IEND,THIS INDICATES possibility of further steps'
         WRITE(*,*)  IEND
*
*
         DO 120 I=1,NC
            WRITE(*,*) L1(I),L2(I),L3(I),L4(I),L5(I)
 120     CONTINUE
*
        END
```